

1-Bromopyrene

Other names:	pyrene, 1-bromo-
Inchi:	InChI=1S/C16H9Br/c17-14-9-7-12-5-4-10-2-1-3-11-6-8-13(14)16(12)15(10)11/h1-9H
InchiKey:	HYGLETVERPVXOS-UHFFFAOYSA-N
Formula:	C16H9Br
SMILES:	BrC1ccc2ccc3cccc4ccc1c2c34
Mol. weight [g/mol]:	281.15
CAS:	1714-29-0

Physical Properties

Property code	Value	Unit	Source
ea	0.72 ± 0.10	eV	NIST Webbook
gf	495.87	kJ/mol	Joback Method
hf	382.63	kJ/mol	Joback Method
hfus	29.39	kJ/mol	Joback Method
hvap	66.19	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	5.346		Crippen Method
mcvol	175.960	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	722.50	K	Joback Method
tc	990.26	K	Joback Method
tf	368.15 ± 2.00	K	NIST Webbook
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.48	J/molxK	722.50	Joback Method
cpg	428.94	J/molxK	767.13	Joback Method
cpg	439.62	J/molxK	811.75	Joback Method
cpg	449.75	J/molxK	856.38	Joback Method
cpg	459.59	J/molxK	901.01	Joback Method
cpg	469.38	J/molxK	945.64	Joback Method
cpg	479.37	J/molxK	990.26	Joback Method

dvisc	0.0024437	Paxs	498.24	Joback Method
dvisc	0.0021977	Paxs	535.62	Joback Method
dvisc	0.0020039	Paxs	572.99	Joback Method
dvisc	0.0018480	Paxs	610.37	Joback Method
dvisc	0.0017203	Paxs	647.75	Joback Method
dvisc	0.0016139	Paxs	685.12	Joback Method
dvisc	0.0015242	Paxs	722.50	Joback Method
hsubt	99.20 ± 4.40	kJ/mol	344.50	NIST Webbook
psub	1.80e-04	kPa	365.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.60e-04	kPa	363.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	2.33e-04	kPa	367.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.28e-04	kPa	363.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	1.55e-04	kPa	363.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.12e-04	kPa	362.30	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	9.01e-05	kPa	358.60	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	7.83e-05	kPa	358.30	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	6.06e-05	kPa	355.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	5.94e-05	kPa	355.30	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	4.97e-05	kPa	353.80	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	5.08e-05	kPa	353.80	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	5.08e-05	kPa	351.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	2.82e-05	kPa	347.30	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	3.08e-05	kPa	347.10	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.37e-05	kPa	339.50	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.52e-05	kPa	339.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.80e-06	kPa	320.80	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique: <https://www.doi.org/10.1016/j.jct.2007.09.006>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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