Naphthalene, 1,4-dibromo-

Other names: 1,4-dibromonaphthalene
Inchi: InChI=1S/C10H6Br2/c11-9-5-6-10(12)8-4-2-1-3-7(8)9/h1-6H
InchiKey: IBGUDZMIAZLJNY-UHFFFAOYSA-N
Formula: C10H6Br2
SMILES: Brc1ccc(Br)c2ccccc12
Mol. weight [g/mol]: 285.96
CAS: 83-53-4

Physical Properties

Property code	Value	Unit	Source
gf	261.76	kJ/mol	Joback Method
hf	207.59	kJ/mol	Joback Method
hfus	22.51	kJ/mol	Joback Method
hvap	55.96	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.365		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	4480.21	kPa	Joback Method
tb	616.14	K	Joback Method
tc	886.97	K	Joback Method
tf	406.22	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.60	J/mol×K	886.97	Joback Method
cpg	283.96	J/mol×K	661.28	Joback Method
cpg	293.09	J/mol×K	706.42	Joback Method
cpg	301.39	J/mol×K	751.56	Joback Method
cpg	308.99	J/mol×K	796.69	Joback Method
cpg	316.02	J/mol×K	841.83	Joback Method
cpg	273.88	J/mol×K	616.14	Joback Method
dvisc	0.0013543	Pa×s	406.22	Joback Method

dvisc	0.0010195	Pa×s	441.21	Joback Method
dvisc	0.0008001	Pa×s	476.19	Joback Method
dvisc	0.0006491	Pa×s	511.18	Joback Method
dvisc	0.0005409	Pa×s	546.17	Joback Method
dvisc	0.0004608	Pa×s	581.15	Joback Method
dvisc	0.0003997	Pa×s	616.14	Joback Method
hsubt	90.80 ± 1.70	kJ/mol	309.50	NIST Webbook
psub	1.93e-05	kPa	297.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.95e-05	kPa	297.80	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	2.88e-05	kPa	301.20	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	3.84e-05	kPa	303.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	4.45e-05	kPa	304.60	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	
psub	5.99e-05	kPa	306.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	
psub	6.88e-05	kPa	307.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	
psub	1.27e-04	kPa	313.50	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	
psub	2.25e-04	kPa	318.80	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	

psub	2.69e-04	kPa	320.60	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	3.25e-04	kPa	322.70	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83534&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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