1-BROMO-4-PROPYLBENZENE

Inchi: InChI=1S/C9H11Br/c1-2-3-8-4-6-9(10)7-5-8/h4-7H,2-3H2,1H3
InchiKey: NUPWGLKBGVNSJX-UHFFFAOYSA-N
Formula: C9H11Br
SMILES: CCCc1ccc(Br)cc1
Mol. weight [g/mol]: 199.09
CAS: 588-93-2

Physical Properties

Property code	Value	Unit	Source
af	0.3942		Cheméo Relay (1.0)
gf	142.00	kJ/mol	Joback Method
hf	30.25	kJ/mol	Cheméo Relay (1.0)
hfus	18.00	kJ/mol	Joback Method
hvap	57.02	kJ/mol	Cheméo Relay (1.0)
ie	8.67	eV	Cheméo Relay (1.0)
log10ws	-4.38		Cheméo Relay (1.0)
logp	3.402		Crippen Method
mcvol	131.410	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
tb	502.14	K	Cheméo Relay (1.0)
tc	702.63	K	Cheméo Relay (1.0)
tf	253.66	K	Cheméo Relay (1.0)
vc	0.481	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.70	J/mol×K	503.14	Joback Method
cpg	267.58	J/mol×K	540.79	Joback Method
cpg	279.63	J/mol×K	578.44	Joback Method
cpg	290.91	J/mol×K	616.09	Joback Method
cpg	301.45	J/mol×K	653.74	Joback Method
cpg	311.30	J/mol×K	691.39	Joback Method
cpg	320.49	J/mol×K	729.04	Joback Method

dvisc	0.0021703	Pa×s	289.93	Joback Method
dvisc	0.0012691	Pa×s	325.47	Joback Method
dvisc	0.0008248	Pa×s	361.00	Joback Method
dvisc	0.0005791	Pa×s	396.53	Joback Method
dvisc	0.0004309	Pa×s	432.07	Joback Method
dvisc	0.0003354	Pa×s	467.61	Joback Method
dvisc	0.0002705	Pa×s	503.14	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41588e+01
Coeff. B	-3.99330e+03
Coeff. C	-7.96360e+01
Temperature range (K), min.	367.52
Temperature range (K), max.	530.99

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C588932&Units=SI

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

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor

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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume