DL-2,3-Dibromobutane

Other names: Erythro-2,3-dibromobutane
Inchi: InChI=1S/C4H8Br2/c1-3(5)4(2)6/h3-4H,1-2H3
InchiKey: BXXWFOGWXLJPPA-UHFFFAOYSA-N
Formula: C4H8Br2
SMILES: CC(Br)C(C)Br
Mol. weight [g/mol]: 215.91
CAS: 598-71-0

Physical Properties

Property code	Value	Unit	Source
gf	6.56	kJ/mol	Joback Method
hf	-102.90	kJ/mol	NIST Webbook
hfus	9.64	kJ/mol	Joback Method
hvap	46.99	kJ/mol	NIST Webbook
ie	10.12	eV	NIST Webbook
log10ws	-2.58		Crippen Method
logp	2.553		Crippen Method
mcvol	102.220	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
tb	422.36	K	Joback Method
tc	639.11	K	Joback Method
tf	224.44	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.90	J/mol×K	639.11	Joback Method
cpg	194.90	J/mol×K	602.98	Joback Method
cpg	188.50	J/mol×K	566.86	Joback Method
cpg	181.67	J/mol×K	530.73	Joback Method
cpg	174.37	J/mol×K	494.61	Joback Method
cpg	166.58	J/mol×K	458.48	Joback Method
cpg	158.26	J/mol×K	422.36	Joback Method

dvisc	0.0065317	Pa×s	224.44	Joback Method
dvisc	0.0004045	Pa×s	422.36	Joback Method
dvisc	0.0005285	Pa×s	389.37	Joback Method
dvisc	0.0007254	Pa×s	356.39	Joback Method
dvisc	0.0010621	Pa×s	323.40	Joback Method
dvisc	0.0016958	Pa×s	290.41	Joback Method
dvisc	0.0030527	Pa×s	257.43	Joback Method
hvapt	40.90	kJ/mol	356.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41108e+01
Coeff. B	-3.10284e+03
Coeff. C	-1.06927e+02
Temperature range (K), min.	331.39
Temperature range (K), max.	459.55

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C598710&Units=SI

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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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