2,3-Dibromo-1,4-dichlorobutane

Inchi: InChI=1S/C4H6Br2Cl2/c5-3(1-7)4(6)2-8/h3-4H,1-2H2
InchiKey: FPPZFTLHBVZMCA-UHFFFAOYSA-N
Formula: C4H6Br2Cl2
SMILES: ClCC(Br)C(Br)CCl
Mol. weight [g/mol]: 284.80
CAS: 4911-46-0

Physical Properties

Property code	Value	Unit	Source
gf	-17.30	kJ/mol	Joback Method
hf	-115.27	kJ/mol	Joback Method
hfus	18.03	kJ/mol	Joback Method
hvap	45.36	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.991		Crippen Method
mcvol	126.700	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
tb	497.22	K	Joback Method
tc	726.83	K	Joback Method
tf	284.28	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.56	J/mol×K	497.22	Joback Method
cpg	206.70	J/mol×K	535.49	Joback Method
cpg	213.29	J/mol×K	573.76	Joback Method
cpg	219.37	J/mol×K	612.03	Joback Method
cpg	224.97	J/mol×K	650.29	Joback Method
cpg	230.15	J/mol×K	688.56	Joback Method
cpg	234.94	J/mol×K	726.83	Joback Method
dvisc	0.0045784	Pa×s	284.28	Joback Method
dvisc	0.0023808	Pa×s	319.77	Joback Method

dvisc	0.0014109	Pa×s	355.26	Joback Method
dvisc	0.0009194	Pa×s	390.75	Joback Method
dvisc	0.0006434	Pa×s	426.24	Joback Method
dvisc	0.0004757	Pa×s	461.73	Joback Method
dvisc	0.0003672	Pa×s	497.22	Joback Method

Sources

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=C4911460&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume