1-Bromo-2,3-dichlorobutane

Inchi: InChI=1S/C4H7BrCl2/c1-3(6)4(7)2-5/h3-4H,2H2,1H3
InchiKey: KXJKILOJEOGJHV-UHFFFAOYSA-N
Formula: C4H7BrCl2
SMILES: CC(Cl)C(Cl)CBr
Mol. weight [g/mol]: 205.91
CAS: 38585-79-4

Physical Properties

Property code	Value	Unit	Source
gf	-31.62	kJ/mol	Joback Method
hf	-141.60	kJ/mol	Joback Method
hfus	12.75	kJ/mol	Joback Method
hvap	38.93	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.616		Crippen Method
mcvol	109.200	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
tb	431.06	K	Joback Method
tc	642.82	K	Joback Method
tf	224.48	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.69	J/mol×K	431.06	Joback Method
cpg	179.45	J/mol×K	466.35	Joback Method
cpg	186.74	J/mol×K	501.65	Joback Method
cpg	193.58	J/mol×K	536.94	Joback Method
cpg	199.99	J/mol×K	572.23	Joback Method
cpg	206.00	J/mol×K	607.53	Joback Method
cpg	211.62	J/mol×K	642.82	Joback Method
dvisc	0.0075075	Pa×s	224.48	Joback Method
dvisc	0.0032950	Pa×s	258.91	Joback Method

dvisc	0.0017545	Pa×s	293.34	Joback Method
dvisc	0.0010665	Pa×s	327.77	Joback Method
dvisc	0.0007127	Pa×s	362.20	Joback Method
dvisc	0.0005107	Pa×s	396.63	Joback Method
dvisc	0.0003860	Pa×s	431.06	Joback Method

Sources

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=C38585794&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
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