Dimethyl 2-chloro-3-bromobutanedioate

Inchi: InChI=1S/C6H6BrClO4/c1-11-5(9)3(7)4(8)6(10)12-2/h1-2H3/b4-3+
InchiKey: QSVNSPIQPOWBRG-ONEGZZNKSA-N
Formula: C6H6BrClO4
SMILES: COC(=O)C(Cl)=C(Br)C(=O)OC
Mol. weight [g/mol]: 257.47

Physical Properties

Property code	Value	Unit	Source
gf	-402.69	kJ/mol	Joback Method
hf	-548.54	kJ/mol	Joback Method
hfus	23.93	kJ/mol	Joback Method
hvap	58.20	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.178		Crippen Method
mcvol	135.720	ml/mol	McGowan Method
pc	3867.48	kPa	Joback Method
rinpol	1406.00		NIST Webbook
tb	596.77	K	Joback Method
tc	819.40	K	Joback Method
tf	358.42	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.04	J/mol×K	596.77	Joback Method
cpg	276.89	J/mol×K	633.88	Joback Method
cpg	284.26	J/mol×K	670.98	Joback Method
cpg	291.17	J/mol×K	708.09	Joback Method
cpg	297.62	J/mol×K	745.19	Joback Method
cpg	303.61	J/mol×K	782.30	Joback Method
cpg	309.16	J/mol×K	819.40	Joback Method

Sources

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=R80255&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume