

2,3-Butanediol, bis(alpha,alpha-di-chloropropionate)

Inchi:	InChI=1S/C10H14Cl4O4/c1-5(17-7(15)9(3,11)12)6(2)18-8(16)10(4,13)14/h5-6H,1-4H3
InchiKey:	PTNMCSYWAFVACY-UHFFFAOYSA-N
Formula:	C10H14Cl4O4
SMILES:	CC(OC(=O)C(C)(Cl)Cl)C(C)OC(=O)C(C)(Cl)Cl
Mol. weight [g/mol]:	340.03
CAS:	124715-84-0

Physical Properties

Property code	Value	Unit	Source
gf	-481.44	kJ/mol	Joback Method
hf	-830.35	kJ/mol	Joback Method
hfus	22.14	kJ/mol	Joback Method
hvap	70.34	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.237		Crippen Method
mcvol	215.600	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
tb	723.16	K	Joback Method
tc	945.70	K	Joback Method
tf	441.30	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.83	J/molxK	723.16	Joback Method
cpg	535.85	J/molxK	760.25	Joback Method
cpg	545.97	J/molxK	797.34	Joback Method
cpg	555.23	J/molxK	834.43	Joback Method
cpg	563.68	J/molxK	871.52	Joback Method
cpg	571.37	J/molxK	908.61	Joback Method
cpg	578.34	J/molxK	945.70	Joback Method
dvisc	0.0012705	Paxs	441.30	Joback Method
dvisc	0.0006282	Paxs	488.28	Joback Method

dvisc	0.0003515	Paxs	535.25	Joback Method
dvisc	0.0002160	Paxs	582.23	Joback Method
dvisc	0.0001427	Paxs	629.21	Joback Method
dvisc	0.0000999	Paxs	676.18	Joback Method
dvisc	0.0000733	Paxs	723.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C124715840&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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