3-CHLORO-2,2-BIS(CHLOROMETHYL)PROPANOIC ACID

Other names: 3-Chloro-2,2-bis(chloromethyl)propionic acid
Inchi: InChI=1S/C5H7Cl3O2/c6-1-5(2-7,3-8)4(9)10/h1-3H2,(H,9,10)
InchiKey: RDRNKIGGASXJAX-UHFFFAOYSA-N
Formula: C5H7Cl3O2
SMILES: O=C(O)C(CCl)(CCl)CCl
Mol. weight [g/mol]: 205.47

Physical Properties

Property code	Value	Unit	Source
hf	-536.37	kJ/mol	Cheméo Relay (1.0)
hfus	19.57	kJ/mol	Joback Method
ie	10.35	eV	Cheméo Relay (1.0)
log10ws	-1.81		Cheméo Relay (1.0)
logp	1.774		Crippen Method
mcvol	125.470	ml/mol	McGowan Method
tb	538.12	K	Cheméo Relay (1.0)
tf	424.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.41	J/mol×K	734.70	Joback Method
cpg	286.08	J/mol×K	767.86	Joback Method
cpg	258.72	J/mol×K	602.07	Joback Method
cpg	265.05	J/mol×K	635.23	Joback Method
cpg	270.93	J/mol×K	668.38	Joback Method
cpg	276.37	J/mol×K	701.54	Joback Method
cpg	251.89	J/mol×K	568.91	Joback Method
dvisc	0.0012008	Pa×s	422.33	Joback Method
dvisc	0.0026399	Pa×s	385.69	Joback Method
dvisc	0.0068476	Pa×s	349.04	Joback Method
dvisc	0.0006194	Pa×s	458.98	Joback Method
dvisc	0.0003524	Pa×s	495.62	Joback Method
dvisc	0.0002167	Pa×s	532.26	Joback Method

dvisc	0.0001418	Pa×s	568.91	Joback Method
hfust	20.90	kJ/mol	383.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17831708&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point