

3,3-Dichlorobutanoic acid, methyl ester

Inchi:	InChI=1S/C5H8Cl2O2/c1-5(6,7)3-4(8)9-2/h3H2,1-2H3
InchiKey:	NYIDWPOSGNPCLN-UHFFFAOYSA-N
Formula:	C5H8Cl2O2
SMILES:	COC(=O)CC(C)(Cl)Cl
Mol. weight [g/mol]:	171.02

Physical Properties

Property code	Value	Unit	Source
gf	-263.72	kJ/mol	Joback Method
hf	-431.56	kJ/mol	Joback Method
hfus	12.47	kJ/mol	Joback Method
hvap	43.35	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.743		Crippen Method
mcvol	113.230	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	958.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	949.00		NIST Webbook
tb	461.72	K	Joback Method
tc	666.97	K	Joback Method
tf	280.53	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.59	J/molxK	461.72	Joback Method
cpg	221.52	J/molxK	495.93	Joback Method
cpg	229.94	J/molxK	530.14	Joback Method
cpg	237.86	J/molxK	564.34	Joback Method
cpg	245.30	J/molxK	598.55	Joback Method
cpg	252.27	J/molxK	632.76	Joback Method

cpg	258.80	J/mol×K	666.97	Joback Method
dvisc	0.0037813	Paxs	280.53	Joback Method
dvisc	0.0020747	Paxs	310.73	Joback Method
dvisc	0.0012660	Paxs	340.93	Joback Method
dvisc	0.0008372	Paxs	371.12	Joback Method
dvisc	0.0005892	Paxs	401.32	Joback Method
dvisc	0.0004356	Paxs	431.52	Joback Method
dvisc	0.0003350	Paxs	461.72	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=R152464&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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