

Malonic acid, 2,2-dichloroethyl isobutyl ester

Inchi:	InChI=1S/C9H14Cl2O4/c1-6(2)4-14-8(12)3-9(13)15-5-7(10)11/h6-7H,3-5H2,1-2H3
InchiKey:	ZAUJNOGWYTMRR-UHFFFAOYSA-N
Formula:	C9H14Cl2O4
SMILES:	CC(C)COC(=O)CC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	257.11

Physical Properties

Property code	Value	Unit	Source
gf	-471.68	kJ/mol	Joback Method
hf	-760.73	kJ/mol	Joback Method
hfus	25.99	kJ/mol	Joback Method
hvap	61.93	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.923		Crippen Method
mcvol	177.030	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinqol	1519.00		NIST Webbook
tb	631.88	K	Joback Method
tc	829.29	K	Joback Method
tf	365.35	K	Joback Method
vc	0.673	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.34	J/molxK	631.88	Joback Method
cpg	433.00	J/molxK	664.78	Joback Method
cpg	444.04	J/molxK	697.68	Joback Method
cpg	454.47	J/molxK	730.58	Joback Method
cpg	464.28	J/molxK	763.48	Joback Method
cpg	473.47	J/molxK	796.39	Joback Method
cpg	482.04	J/molxK	829.29	Joback Method
dvisc	0.0022806	Paxs	365.35	Joback Method
dvisc	0.0011482	Paxs	409.77	Joback Method

dvisc	0.0006611	Paxs	454.19	Joback Method
dvisc	0.0004200	Paxs	498.62	Joback Method
dvisc	0.0002874	Paxs	543.04	Joback Method
dvisc	0.0002083	Paxs	587.46	Joback Method
dvisc	0.0001579	Paxs	631.88	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=U349060&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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