

Diethylmalonic acid, 2,2-dichloroethyl isobutyl ester

Inchi:	InChI=1S/C13H22Cl2O4/c1-5-13(6-2,11(16)18-7-9(3)4)12(17)19-8-10(14)15/h9-10H,5-8H
InchiKey:	LYELDPWCLCIULJ-UHFFFAOYSA-N
Formula:	C13H22Cl2O4
SMILES:	CCC(CC)(C(=O)OCC(C)C)C(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	313.22

Physical Properties

Property code	Value	Unit	Source
gf	-435.16	kJ/mol	Joback Method
hf	-852.04	kJ/mol	Joback Method
hfus	28.93	kJ/mol	Joback Method
hvap	69.54	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.339		Crippen Method
mcvol	233.390	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	1671.00		NIST Webbook
tb	720.17	K	Joback Method
tc	918.28	K	Joback Method
tf	412.85	K	Joback Method
vc	0.886	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.09	J/molxK	720.17	Joback Method
cpg	644.32	J/molxK	753.19	Joback Method
cpg	657.66	J/molxK	786.21	Joback Method
cpg	670.13	J/molxK	819.22	Joback Method
cpg	681.77	J/molxK	852.24	Joback Method
cpg	692.59	J/molxK	885.26	Joback Method
cpg	702.61	J/molxK	918.28	Joback Method
dvisc	0.0015816	Paxs	412.85	Joback Method
dvisc	0.0007226	Paxs	464.07	Joback Method

dvisc	0.0003858	Paxs	515.29	Joback Method
dvisc	0.0002307	Paxs	566.51	Joback Method
dvisc	0.0001503	Paxs	617.73	Joback Method
dvisc	0.0001045	Paxs	668.95	Joback Method
dvisc	0.0000765	Paxs	720.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370778&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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