

Diethylmalonic acid, monochloride, 3-methylpent-2-yl ester

Inchi:	InChI=1S/C13H23ClO3/c1-6-9(4)10(5)17-12(16)13(7-2,8-3)11(14)15/h9-10H,6-8H2,1-5H
InchiKey:	ZDDBPJOVXZSLHJ-UHFFFAOYSA-N
Formula:	C13H23ClO3
SMILES:	CCC(C)C(C)OC(=O)C(CC)(CC)C(=O)Cl
Mol. weight [g/mol]:	262.77

Physical Properties

Property code	Value	Unit	Source
gf	-318.23	kJ/mol	Joback Method
hf	-704.08	kJ/mol	Joback Method
hfus	23.55	kJ/mol	Joback Method
hvap	62.75	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.536		Crippen Method
mcvol	215.280	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	1438.00		NIST Webbook
tb	660.32	K	Joback Method
tc	855.72	K	Joback Method
tf	360.70	K	Joback Method
vc	0.820	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.52	J/molxK	660.32	Joback Method
cpg	590.10	J/molxK	692.89	Joback Method
cpg	604.78	J/molxK	725.45	Joback Method
cpg	618.59	J/molxK	758.02	Joback Method
cpg	631.58	J/molxK	790.59	Joback Method
cpg	643.77	J/molxK	823.16	Joback Method
cpg	655.19	J/molxK	855.72	Joback Method
dvisc	0.0032395	Paxs	360.70	Joback Method
dvisc	0.0013318	Paxs	410.64	Joback Method

dvisc	0.0006639	Paxs	460.57	Joback Method
dvisc	0.0003793	Paxs	510.51	Joback Method
dvisc	0.0002394	Paxs	560.45	Joback Method
dvisc	0.0001629	Paxs	610.38	Joback Method
dvisc	0.0001175	Paxs	660.32	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U369745&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
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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