

Diethylmalonic acid, monochloride, 3-methylpentyl ester

Inchi:	InChI=1S/C13H23ClO3/c1-5-10(4)8-9-17-12(16)13(6-2,7-3)11(14)15/h10H,5-9H2,1-4H3
InchiKey:	OQARFENPLCQVQV-UHFFFAOYSA-N
Formula:	C13H23ClO3
SMILES:	CCC(C)CCOC(=O)C(CC)(CC)C(=O)Cl
Mol. weight [g/mol]:	262.77

Physical Properties

Property code	Value	Unit	Source
gf	-315.79	kJ/mol	Joback Method
hf	-698.80	kJ/mol	Joback Method
hfus	27.07	kJ/mol	Joback Method
hvap	63.14	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.538		Crippen Method
mcvol	215.280	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpola	1453.00		NIST Webbook
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tb	660.76	K	Joback Method
tc	852.92	K	Joback Method
tf	375.70	K	Joback Method
vc	0.826	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.05	J/molxK	660.76	Joback Method
cpg	589.33	J/molxK	692.79	Joback Method
cpg	603.76	J/molxK	724.81	Joback Method
cpg	617.36	J/molxK	756.84	Joback Method
cpg	630.17	J/molxK	788.87	Joback Method
cpg	642.21	J/molxK	820.90	Joback Method
cpg	653.51	J/molxK	852.92	Joback Method
dvisc	0.0025016	Paxs	375.70	Joback Method

dvisc	0.0011508	Paxs	423.21	Joback Method
dvisc	0.0006192	Paxs	470.72	Joback Method
dvisc	0.0003733	Paxs	518.23	Joback Method
dvisc	0.0002450	Paxs	565.74	Joback Method
dvisc	0.0001716	Paxs	613.25	Joback Method
dvisc	0.0001266	Paxs	660.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370604&Units=SI
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

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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