

Diethylmalonic acid, 2,2-dichloroethyl tridecyl ester

Inchi:	InChI=1S/C22H40Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-27-20(25)22(5-2,6-3)21(26)
InchiKey:	GDWDGYJVSHNOFN-UHFFFAOYSA-N
Formula:	C22H40Cl2O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	439.46

Physical Properties

Property code	Value	Unit	Source
gf	-356.94	kJ/mol	Joback Method
hf	-1032.52	kJ/mol	Joback Method
hfus	55.77	kJ/mol	Joback Method
hvap	89.96	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.994		Crippen Method
mcvol	360.200	ml/mol	McGowan Method
pc	926.68	kPa	Joback Method
rinsol	2624.00		NIST Webbook
tb	926.53	K	Joback Method
tc	1134.35	K	Joback Method
tf	529.28	K	Joback Method
vc	1.397	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.22	J/molxK	926.53	Joback Method
cpg	1226.60	J/molxK	1099.71	Joback Method
cpg	1214.19	J/molxK	1065.07	Joback Method
cpg	1200.70	J/molxK	1030.44	Joback Method
cpg	1186.08	J/molxK	995.80	Joback Method
cpg	1170.27	J/molxK	961.17	Joback Method
cpg	1237.97	J/molxK	1134.35	Joback Method
dvisc	0.0000198	Paxs	926.53	Joback Method
dvisc	0.0000271	Paxs	860.32	Joback Method

dvisc	0.0000389	Paxs	794.11	Joback Method
dvisc	0.0000596	Paxs	727.90	Joback Method
dvisc	0.0000997	Paxs	661.70	Joback Method
dvisc	0.0001869	Paxs	595.49	Joback Method
dvisc	0.0004101	Paxs	529.28	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=U370788&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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