

Diethylmalonic acid, 2,2-dichloroethyl undecyl ester

Inchi:	InChI=1S/C20H36Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-25-18(23)20(5-2,6-3)19(24)26-16
InchiKey:	RJRYMDYPGVFYFD-UHFFFAOYSA-N
Formula:	C20H36Cl2O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	411.40

Physical Properties

Property code	Value	Unit	Source
gf	-373.78	kJ/mol	Joback Method
hf	-991.24	kJ/mol	Joback Method
hfus	50.59	kJ/mol	Joback Method
hvap	85.51	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	6.214		Crippen Method
mcvol	332.020	ml/mol	McGowan Method
pc	1045.30	kPa	Joback Method
rinpol	2412.00		NIST Webbook
tb	880.77	K	Joback Method
tc	1080.51	K	Joback Method
tf	506.74	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.31	J/molxK	880.77	Joback Method
cpg	1047.64	J/molxK	914.06	Joback Method
cpg	1062.85	J/molxK	947.35	Joback Method
cpg	1076.99	J/molxK	980.64	Joback Method
cpg	1090.09	J/molxK	1013.93	Joback Method
cpg	1102.21	J/molxK	1047.22	Joback Method
cpg	1113.37	J/molxK	1080.51	Joback Method
dvisc	0.0005397	Paxs	506.74	Joback Method
dvisc	0.0002505	Paxs	569.08	Joback Method

dvisc	0.0001353	Paxs	631.42	Joback Method
dvisc	0.0000816	Paxs	693.75	Joback Method
dvisc	0.0000535	Paxs	756.09	Joback Method
dvisc	0.0000374	Paxs	818.43	Joback Method
dvisc	0.0000275	Paxs	880.77	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=U370786&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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