

Diethylmalonic acid, 2,6-dichlorophenyl hexadecyl ester

Inchi:	InChI=1S/C29H46Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-23-34-27(32)29(5-2
InchiKey:	AHQKHIFNJHYOLU-UHFFFAOYSA-N
Formula:	C29H46Cl2O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	529.58

Physical Properties

Property code	Value	Unit	Source
gf	-202.41	kJ/mol	Joback Method
hf	-958.13	kJ/mol	Joback Method
hfus	70.68	kJ/mol	Joback Method
hvap	109.53	kJ/mol	Joback Method
log10ws	-10.57		Crippen Method
logp	9.730		Crippen Method
mcvol	435.070	ml/mol	McGowan Method
pc	744.88	kPa	Joback Method
rinpol	3431.00		NIST Webbook
rinpol	3431.00		NIST Webbook
tb	1123.77	K	Joback Method
tc	1388.35	K	Joback Method
tf	674.63	K	Joback Method
vc	1.687	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1480.41	J/molxK	1123.77	Joback Method
cpg	1496.77	J/molxK	1167.87	Joback Method
cpg	1511.37	J/molxK	1211.96	Joback Method
cpg	1524.35	J/molxK	1256.06	Joback Method
cpg	1535.86	J/molxK	1300.16	Joback Method
cpg	1546.03	J/molxK	1344.25	Joback Method
cpg	1555.00	J/molxK	1388.35	Joback Method
dvisc	0.0000941	Paxs	674.63	Joback Method

dvisc	0.0000498	Paxs	749.49	Joback Method
dvisc	0.0000296	Paxs	824.34	Joback Method
dvisc	0.0000192	Paxs	899.20	Joback Method
dvisc	0.0000133	Paxs	974.06	Joback Method
dvisc	0.0000097	Paxs	1048.91	Joback Method
dvisc	0.0000074	Paxs	1123.77	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=U369943&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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