

Diethylmalonic acid, 4-chloro-3-methylphenyl tridecyl ester

Inchi:	InChI=1S/C27H43ClO4/c1-5-8-9-10-11-12-13-14-15-16-17-20-31-25(29)27(6-2,7-3)26(30)
InchiKey:	GNOUYVUJJSOMJY-UHFFFAOYSA-N
Formula:	C27H43ClO4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	467.08

Physical Properties

Property code	Value	Unit	Source
gf	-207.32	kJ/mol	Joback Method
hf	-901.11	kJ/mol	Joback Method
hfus	61.31	kJ/mol	Joback Method
hvap	100.70	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.214		Crippen Method
mvol	394.650	ml/mol	McGowan Method
pc	847.51	kPa	Joback Method
rinpol	3045.00		NIST Webbook
rinpol	3045.00		NIST Webbook
tb	1040.58	K	Joback Method
tc	1275.64	K	Joback Method
tf	622.17	K	Joback Method
vc	1.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1331.37	J/molxK	1040.58	Joback Method
cpg	1347.98	J/molxK	1079.76	Joback Method
cpg	1363.05	J/molxK	1118.93	Joback Method
cpg	1376.67	J/molxK	1158.11	Joback Method
cpg	1388.93	J/molxK	1197.29	Joback Method
cpg	1399.91	J/molxK	1236.47	Joback Method
cpg	1409.70	J/molxK	1275.64	Joback Method
dvisc	0.0001590	Paxs	622.17	Joback Method

dvisc	0.0000841	Paxs	691.91	Joback Method
dvisc	0.0000500	Paxs	761.64	Joback Method
dvisc	0.0000324	Paxs	831.38	Joback Method
dvisc	0.0000225	Paxs	901.11	Joback Method
dvisc	0.0000164	Paxs	970.84	Joback Method
dvisc	0.0000125	Paxs	1040.58	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=U369922&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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