

Dimethylmalonic acid, hexadecyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C27H41Cl3O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-33-25(31)27(2,3)26
InchiKey: HRRRBSWPUNKJLD-UHFFFAOYSA-N
Formula: C27H41Cl3O4
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 535.97

Physical Properties

Property code	Value	Unit	Source
gf	-240.81	kJ/mol	Joback Method
hf	-944.06	kJ/mol	Joback Method
hfus	69.31	kJ/mol	Joback Method
hvap	110.13	kJ/mol	Joback Method
log10ws	-10.41		Crippen Method
logp	9.603		Crippen Method
mvol	419.130	ml/mol	McGowan Method
pc	805.25	kPa	Joback Method
rinpol	3381.00		NIST Webbook
rinpol	3381.00		NIST Webbook
tb	1120.42	K	Joback Method
tc	1378.77	K	Joback Method
tf	694.53	K	Joback Method
vc	1.623	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1375.46	J/molxK	1120.42	Joback Method
cpg	1389.74	J/molxK	1163.48	Joback Method
cpg	1402.39	J/molxK	1206.54	Joback Method
cpg	1413.53	J/molxK	1249.60	Joback Method
cpg	1423.26	J/molxK	1292.66	Joback Method
cpg	1431.70	J/molxK	1335.72	Joback Method
cpg	1438.97	J/molxK	1378.77	Joback Method
dvisc	0.0000877	Paxs	694.53	Joback Method

dvisc	0.0000499	Paxs	765.51	Joback Method
dvisc	0.0000312	Paxs	836.49	Joback Method
dvisc	0.0000210	Paxs	907.48	Joback Method
dvisc	0.0000150	Paxs	978.46	Joback Method
dvisc	0.0000112	Paxs	1049.44	Joback Method
dvisc	0.0000087	Paxs	1120.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363658&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

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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