

Diethylmalonic acid, 2,4-dichlorophenyl tetradecyl ester

Inchi:	InChI=1S/C27H42Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-20-32-25(30)27(5-2,6-3)26
InchiKey:	RIDDGGUKLQODCP-UHFFFAOYSA-N
Formula:	C27H42Cl2O4
SMILES:	CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	501.53

Physical Properties

Property code	Value	Unit	Source
gf	-219.25	kJ/mol	Joback Method
hf	-916.85	kJ/mol	Joback Method
hfus	65.50	kJ/mol	Joback Method
hvap	105.08	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	8.950		Crippen Method
mcvol	406.890	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
rinpol	3217.00		NIST Webbook
rinpol	3217.00		NIST Webbook
tb	1078.01	K	Joback Method
tc	1323.54	K	Joback Method
tf	652.09	K	Joback Method
vc	1.575	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1355.04	J/molxK	1078.01	Joback Method
cpg	1370.60	J/molxK	1118.93	Joback Method
cpg	1384.60	J/molxK	1159.85	Joback Method
cpg	1397.16	J/molxK	1200.77	Joback Method
cpg	1408.37	J/molxK	1241.69	Joback Method
cpg	1418.34	J/molxK	1282.61	Joback Method
cpg	1427.16	J/molxK	1323.54	Joback Method
dvisc	0.0001238	Paxs	652.09	Joback Method

dvisc	0.0000668	Paxs	723.08	Joback Method
dvisc	0.0000402	Paxs	794.06	Joback Method
dvisc	0.0000263	Paxs	865.05	Joback Method
dvisc	0.0000184	Paxs	936.04	Joback Method
dvisc	0.0000135	Paxs	1007.02	Joback Method
dvisc	0.0000103	Paxs	1078.01	Joback Method

Sources

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=U369576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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