Diethylmalonic acid, decyl 2,4-dichloronaphth-1-yl ester

Inchi: InChI=1S/C27H36Cl2O4/c1-4-7-8-9-10-11-12-15-18-32-25(30)27(5-2,6-3)26(31)33-24-21

InchiKey: LKFIVNZIFASHNK-UHFFFAOYSA-N

Formula: C27H36Cl2O4

SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)c2ccccc12

Mol. weight [g/mol]: 495.48

Physical Properties

Property code	Value	Unit	Source
gf	-122.23	kJ/mol	Joback Method
hf	-737.25	kJ/mol	Joback Method
hfus	62.13	kJ/mol	Joback Method
hvap	107.38	kJ/mol	Joback Method
log10ws	-9.86		Crippen Method
logp	8.542		Crippen Method
mcvol	387.430	ml/mol	McGowan Method
pc	951.42	kPa	Joback Method
rinpol	3362.00		NIST Webbook
tb	1101.97	K	Joback Method
tc	1349.63	K	Joback Method
tf	697.31	K	Joback Method
vc	1.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1268.14	J/mol×K	1101.97	Joback Method
cpg	1282.60	J/mol×K	1143.25	Joback Method
cpg	1295.97	J/mol×K	1184.52	Joback Method
cpg	1308.37	J/mol×K	1225.80	Joback Method
cpg	1319.93	J/mol×K	1267.07	Joback Method
cpg	1330.77	J/mol×K	1308.35	Joback Method
cpg	1341.04	J/mol×K	1349.63	Joback Method
dvisc	0.0001664	Pa×s	697.31	Joback Method
dvisc	0.0001035	Pa×s	764.75	Joback Method

dvisc	0.0000695	Pa×s	832.20	Joback Method
dvisc	0.0000496	Pa×s	899.64	Joback Method
dvisc	0.0000371	Pa×s	967.08	Joback Method
dvisc	0.0000288	Pa×s	1034.53	Joback Method
dvisc	0.0000230	Pa×s	1101.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370058&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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