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

Inchi: InChI=1S/C28H38Cl2O4/c1-4-7-8-9-10-11-12-13-16-19-33-26(31)28(5-2,6-3)27(32)34-25
InchiKey: ODTJGKPISYMQJS-UHFFFAOYSA-N
Formula: C28H38Cl2O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)c2ccccc12
Mol. weight [g/mol]: 509.50

Physical Properties

Property code	Value	Unit	Source
gf	-113.81	kJ/mol	Joback Method
hf	-757.89	kJ/mol	Joback Method
hfus	64.72	kJ/mol	Joback Method
hvap	109.61	kJ/mol	Joback Method
log10ws	-10.28		Crippen Method
logp	8.932		Crippen Method
mcvol	401.520	ml/mol	McGowan Method
pc	897.49	kPa	Joback Method
rinpol	3474.00		NIST Webbook
rinpol	3474.00		NIST Webbook
tb	1124.85	K	Joback Method
tc	1379.37	K	Joback Method
tf	708.58	K	Joback Method
vc	1.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1330.36	J/mol×K	1124.85	Joback Method
cpg	1345.30	J/mol×K	1167.27	Joback Method
cpg	1359.11	J/mol×K	1209.69	Joback Method
cpg	1371.94	J/mol×K	1252.11	Joback Method
cpg	1383.94	J/mol×K	1294.53	Joback Method
cpg	1395.24	J/mol×K	1336.95	Joback Method
cpg	1406.00	J/mol×K	1379.37	Joback Method
dvisc	0.0001470	Pa×s	708.58	Joback Method

dvisc	0.0000906	Pa×s	777.96	Joback Method
dvisc	0.0000604	Pa×s	847.34	Joback Method
dvisc	0.0000428	Pa×s	916.71	Joback Method
dvisc	0.0000319	Pa×s	986.09	Joback Method
dvisc	0.0000247	Pa×s	1055.47	Joback Method
dvisc	0.0000197	Pa×s	1124.85	Joback Method

Sources

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=U370059&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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