Diethylmalonic acid, 2,4-dichloronaphth-1-yl 2-methylhex-3-yl ester

Inchi: InChI=1S/C24H30Cl2O4/c1-6-11-20(15(4)5)29-22(27)24(7-2,8-3)23(28)30-21-17-13-10-9

InchiKey: ICMQCEBOUMLQAL-UHFFFAOYSA-N

Formula: C24H30Cl2O4

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

Mol. weight [g/mol]: 453.40

Physical Properties

Property code	Value	Unit	Source
gf	-152.37	kJ/mol	Joback Method
hf	-685.89	kJ/mol	Joback Method
hfus	47.32	kJ/mol	Joback Method
hvap	99.93	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.226		Crippen Method
mcvol	345.160	ml/mol	McGowan Method
pc	1158.50	kPa	Joback Method
rinpol	2914.00		NIST Webbook
rinpol	2914.00		NIST Webbook
tb	1032.45	K	Joback Method
tc	1268.50	K	Joback Method
tf	633.50	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.04	J/mol×K	1032.45	Joback Method
cpg	1098.33	J/mol×K	1071.79	Joback Method
cpg	1110.54	J/mol×K	1111.13	Joback Method
cpg	1121.77	J/mol×K	1150.48	Joback Method
cpg	1132.12	J/mol×K	1189.82	Joback Method
cpg	1141.69	J/mol×K	1229.16	Joback Method
cpg	1150.57	J/mol×K	1268.50	Joback Method
dvisc	0.0002626	Pa×s	633.50	Joback Method

dvisc	0.0001542	Pa×s	699.99	Joback Method
dvisc	0.0000994	Pa×s	766.48	Joback Method
dvisc	0.0000687	Pa×s	832.98	Joback Method
dvisc	0.0000501	Pa×s	899.47	Joback Method
dvisc	0.0000382	Pa×s	965.96	Joback Method
dvisc	0.0000302	Pa×s	1032.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370053&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

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