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

Inchi: InChI=1S/C22H26Cl2O4/c1-4-7-10-13-27-20(25)22(5-2,6-3)21(26)28-19-16-12-9-8-11-15

InchiKey: IPUBKCSOFFDYQO-UHFFFAOYSA-N

Formula: C22H26Cl2O4

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

Mol. weight [g/mol]: 425.35

Physical Properties

Property code	Value	Unit	Source
gf	-164.33	kJ/mol	Joback Method
hf	-634.05	kJ/mol	Joback Method
hfus	49.18	kJ/mol	Joback Method
hvap	96.25	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	6.592		Crippen Method
mcvol	316.980	ml/mol	McGowan Method
pc	1310.85	kPa	Joback Method
rinpol	2881.00		NIST Webbook
tb	987.57	K	Joback Method
tc	1217.90	K	Joback Method
tf	640.96	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.69	J/mol×K	987.57	Joback Method
cpg	977.48	J/mol×K	1025.96	Joback Method
cpg	989.27	J/mol×K	1064.35	Joback Method
cpg	1000.14	J/mol×K	1102.74	Joback Method
cpg	1010.18	J/mol×K	1141.13	Joback Method
cpg	1019.46	J/mol×K	1179.51	Joback Method
cpg	1028.07	J/mol×K	1217.90	Joback Method
dvisc	0.0002976	Pa×s	640.96	Joback Method
dvisc	0.0001948	Pa×s	698.73	Joback Method

dvisc	0.0001361	Pa×s	756.50	Joback Method
dvisc	0.0001000	Pa×s	814.26	Joback Method
dvisc	0.0000766	Pa×s	872.03	Joback Method
dvisc	0.0000606	Pa×s	929.80	Joback Method
dvisc	0.0000493	Pa×s	987.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370052&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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