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

Inchi: InChI=1S/C21H24Cl2O4/c1-5-21(6-2,19(24)26-12-13(3)4)20(25)27-18-15-10-8-7-9-14(15

InchiKey: GVOCHXTVEHZLCI-UHFFFAOYSA-N

Formula: C21H24Cl2O4

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

Mol. weight [g/mol]: 411.32

Physical Properties

Property code	Value	Unit	Source
gf	-175.19	kJ/mol	Joback Method
hf	-618.69	kJ/mol	Joback Method
hfus	43.07	kJ/mol	Joback Method
hvap	93.64	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	6.058		Crippen Method
mcvol	302.890	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2744.00		NIST Webbook
rinpol	2744.00		NIST Webbook
tb	964.25	K	Joback Method
tc	1196.11	K	Joback Method
tf	614.69	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.21	J/mol×K	964.25	Joback Method
cpg	959.70	J/mol×K	1157.47	Joback Method
cpg	950.73	J/mol×K	1118.82	Joback Method
cpg	940.98	J/mol×K	1080.18	Joback Method
cpg	930.36	J/mol×K	1041.54	Joback Method
cpg	918.80	J/mol×K	1002.89	Joback Method
cpg	967.97	J/mol×K	1196.11	Joback Method
dvisc	0.0000520	Pa×s	964.25	Joback Method

dvisc	0.0000645	Pa×s	905.99	Joback Method
dvisc	0.0000824	Pa×s	847.73	Joback Method
dvisc	0.0001091	Pa×s	789.47	Joback Method
dvisc	0.0001511	Pa×s	731.21	Joback Method
dvisc	0.0002214	Pa×s	672.95	Joback Method
dvisc	0.0003488	Pa×s	614.69	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=U370050&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