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

Inchi: InChI=1S/C20H22Cl2O4/c1-4-11-25-18(23)20(5-2,6-3)19(24)26-17-14-10-8-7-9-13(14)15

InchiKey: XPLQKVHODHWSLY-UHFFFAOYSA-N

Formula: C20H22Cl2O4

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

Mol. weight [g/mol]: 397.29

Physical Properties

Property code	Value	Unit	Source
gf	-181.17	kJ/mol	Joback Method
hf	-592.77	kJ/mol	Joback Method
hfus	44.00	kJ/mol	Joback Method
hvap	91.80	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	5.812		Crippen Method
mcvol	288.800	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2703.00		NIST Webbook
rinpol	2703.00		NIST Webbook
tb	941.81	K	Joback Method
tc	1171.95	K	Joback Method
tf	618.42	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.52	J/mol×K	941.81	Joback Method
cpg	859.80	J/mol×K	980.17	Joback Method
cpg	871.10	J/mol×K	1018.52	Joback Method
cpg	881.49	J/mol×K	1056.88	Joback Method
cpg	891.05	J/mol×K	1095.24	Joback Method
cpg	899.85	J/mol×K	1133.59	Joback Method
cpg	907.96	J/mol×K	1171.95	Joback Method
dvisc	0.0003678	Pa×s	618.42	Joback Method

dvisc	0.0002463	Pa×s	672.32	Joback Method
dvisc	0.0001750	Pa×s	726.22	Joback Method
dvisc	0.0001303	Pa×s	780.12	Joback Method
dvisc	0.0001009	Pa×s	834.01	Joback Method
dvisc	0.0000805	Pa×s	887.91	Joback Method
dvisc	0.0000660	Pa×s	941.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370049&Units=SI

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