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

Inchi: InChI=1S/C26H34Cl2O4/c1-4-7-8-9-10-11-14-17-31-24(29)26(5-2,6-3)25(30)32-23-20-16
InchiKey: UXHJMDWVBMGHFP-UHFFFAOYSA-N
Formula: C26H34Cl2O4
SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)c2ccccc12
Mol. weight [g/mol]: 481.45

Physical Properties

Property code	Value	Unit	Source
gf	-130.65	kJ/mol	Joback Method
hf	-716.61	kJ/mol	Joback Method
hfus	59.54	kJ/mol	Joback Method
hvap	105.16	kJ/mol	Joback Method
log10ws	-9.44		Crippen Method
logp	8.152		Crippen Method
mcvol	373.340	ml/mol	McGowan Method
pc	1010.37	kPa	Joback Method
rinpol	3267.00		NIST Webbook
rinpol	3267.00		NIST Webbook
tb	1079.09	K	Joback Method
tc	1321.11	K	Joback Method
tf	686.04	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.40	J/mol×K	1079.09	Joback Method
cpg	1220.44	J/mol×K	1119.43	Joback Method
cpg	1233.42	J/mol×K	1159.76	Joback Method
cpg	1245.44	J/mol×K	1200.10	Joback Method
cpg	1256.62	J/mol×K	1240.44	Joback Method
cpg	1267.07	J/mol×K	1280.78	Joback Method
cpg	1276.91	J/mol×K	1321.11	Joback Method
dvisc	0.0001879	Pa×s	686.04	Joback Method

dvisc	0.0001180	Pa×s	751.55	Joback Method
dvisc	0.0000799	Pa×s	817.06	Joback Method
dvisc	0.0000573	Pa×s	882.56	Joback Method
dvisc	0.0000430	Pa×s	948.07	Joback Method
dvisc	0.0000335	Pa×s	1013.58	Joback Method
dvisc	0.0000269	Pa×s	1079.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370057&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