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

Inchi: InChI=1S/C25H32Cl2O4/c1-4-7-8-9-10-13-16-30-23(28)25(5-2,6-3)24(29)31-22-19-15-12

InchiKey: HKSMHCMSTVUKHM-UHFFFAOYSA-N

Formula: C25H32Cl2O4

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

Mol. weight [g/mol]: 467.43

Physical Properties

Property code	Value	Unit	Source
gf	-139.07	kJ/mol	Joback Method
hf	-695.97	kJ/mol	Joback Method
hfus	56.95	kJ/mol	Joback Method
hvap	102.93	kJ/mol	Joback Method
log10ws	-9.02		Crippen Method
logp	7.762		Crippen Method
mcvol	359.250	ml/mol	McGowan Method
pc	1074.98	kPa	Joback Method
rinpol	3174.00		NIST Webbook
tb	1056.21	K	Joback Method
tc	1293.75	K	Joback Method
tf	674.77	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1145.15	J/mol×K	1056.21	Joback Method
cpg	1158.82	J/mol×K	1095.80	Joback Method
cpg	1171.46	J/mol×K	1135.39	Joback Method
cpg	1183.14	J/mol×K	1174.98	Joback Method
cpg	1193.99	J/mol×K	1214.57	Joback Method
cpg	1204.10	J/mol×K	1254.16	Joback Method
cpg	1213.59	J/mol×K	1293.75	Joback Method
dvisc	0.0002116	Pa×s	674.77	Joback Method
dvisc	0.0001343	Pa×s	738.34	Joback Method

dvisc	0.0000916	Pa×s	801.92	Joback Method
dvisc	0.0000660	Pa×s	865.49	Joback Method
dvisc	0.0000498	Pa×s	929.06	Joback Method
dvisc	0.0000390	Pa×s	992.64	Joback Method
dvisc	0.0000314	Pa×s	1056.21	Joback Method

Sources

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=U370056&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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