Diethylmalonic acid, 2,3-dichlorophenyl octyl ester

Inchi: InChI=1S/C21H30Cl2O4/c1-4-7-8-9-10-11-15-26-19(24)21(5-2,6-3)20(25)27-17-14-12-13

InchiKey: SPCNDDUQNXXDNZ-UHFFFAOYSA-N

Formula: C21H30Cl2O4

SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 417.37

Physical Properties

Property code	Value	Unit	Source
gf	-269.77	kJ/mol	Joback Method
hf	-793.01	kJ/mol	Joback Method
hfus	49.96	kJ/mol	Joback Method
hvap	91.73	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.609		Crippen Method
mcvol	322.350	ml/mol	McGowan Method
pc	1192.35	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	940.73	K	Joback Method
tc	1157.76	K	Joback Method
tf	584.47	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.86	J/mol×K	940.73	Joback Method
cpg	1002.86	J/mol×K	976.90	Joback Method
cpg	1015.68	J/mol×K	1013.07	Joback Method
cpg	1027.37	J/mol×K	1049.25	Joback Method
cpg	1037.98	J/mol×K	1085.42	Joback Method
cpg	1047.56	J/mol×K	1121.59	Joback Method
cpg	1056.16	J/mol×K	1157.76	Joback Method
dvisc	0.0002679	Pa×s	584.47	Joback Method

dvisc	0.0001533	Pa×s	643.85	Joback Method
dvisc	0.0000964	Pa×s	703.22	Joback Method
dvisc	0.0000651	Pa×s	762.60	Joback Method
dvisc	0.0000466	Pa×s	821.98	Joback Method
dvisc	0.0000349	Pa×s	881.35	Joback Method
dvisc	0.0000271	Pa×s	940.73	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=U370036&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