Diethylmalonic acid, decyl 2,6-dichlorophenyl ester

Inchi: InChI=1S/C23H34Cl2O4/c1-4-7-8-9-10-11-12-13-17-28-21(26)23(5-2,6-3)22(27)29-20-18

InchiKey: JGNJAFXDVOXROC-UHFFFAOYSA-N

Formula: C23H34Cl2O4

SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cccc1Cl

Mol. weight [g/mol]: 445.42

Physical Properties

Property code	Value	Unit	Source
gf	-252.93	kJ/mol	Joback Method
hf	-834.29	kJ/mol	Joback Method
hfus	55.14	kJ/mol	Joback Method
hvap	96.18	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.389		Crippen Method
mcvol	350.530	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	2791.00		NIST Webbook
rinpol	2791.00		NIST Webbook
tb	986.49	K	Joback Method
tc	1208.86	K	Joback Method
tf	607.01	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.95	J/mol×K	986.49	Joback Method
cpg	1123.37	J/mol×K	1023.55	Joback Method
cpg	1136.52	J/mol×K	1060.61	Joback Method
cpg	1148.46	J/mol×K	1097.67	Joback Method
cpg	1159.26	J/mol×K	1134.74	Joback Method
cpg	1168.97	J/mol×K	1171.80	Joback Method
cpg	1177.65	J/mol×K	1208.86	Joback Method
dvisc	0.0002092	Pa×s	607.01	Joback Method

dvisc	0.0001172	Pa×s	670.26	Joback Method
dvisc	0.0000726	Pa×s	733.50	Joback Method
dvisc	0.0000485	Pa×s	796.75	Joback Method
dvisc	0.0000344	Pa×s	860.00	Joback Method
dvisc	0.0000255	Pa×s	923.24	Joback Method
dvisc	0.0000197	Pa×s	986.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369938&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

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