Diethylmalonic acid, 3,5-dichlorophenyl hexyl ester

Inchi: InChI=1S/C19H26Cl2O4/c1-4-7-8-9-10-24-17(22)19(5-2,6-3)18(23)25-16-12-14(20)11-15

InchiKey: SUOTWPCEJZSEPV-UHFFFAOYSA-N

Formula: C19H26Cl2O4

SMILES: CCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1

Mol. weight [g/mol]: 389.31

Physical Properties

Property code	Value	Unit	Source
gf	-286.61	kJ/mol	Joback Method
hf	-751.73	kJ/mol	Joback Method
hfus	44.78	kJ/mol	Joback Method
hvap	87.27	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.829		Crippen Method
mcvol	294.170	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook
tb	894.97	K	Joback Method
tc	1110.14	K	Joback Method
tf	561.93	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.23	J/mol×K	894.97	Joback Method
cpg	884.85	J/mol×K	930.83	Joback Method
cpg	897.35	J/mol×K	966.69	Joback Method
cpg	908.78	J/mol×K	1002.56	Joback Method
cpg	919.18	J/mol×K	1038.42	Joback Method
cpg	928.59	J/mol×K	1074.28	Joback Method
cpg	937.05	J/mol×K	1110.14	Joback Method
dvisc	0.0003392	Pa×s	561.93	Joback Method

dvisc	0.0001985	Pa×s	617.44	Joback Method
dvisc	0.0001269	Pa×s	672.94	Joback Method
dvisc	0.0000868	Pa×s	728.45	Joback Method
dvisc	0.0000627	Pa×s	783.96	Joback Method
dvisc	0.0000473	Pa×s	839.46	Joback Method
dvisc	0.0000369	Pa×s	894.97	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=U370440&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