Diethylmalonic acid, 8-chlorooctyl isobutyl ester

Inchi: InChI=1S/C19H35ClO4/c1-5-19(6-2,18(22)24-15-16(3)4)17(21)23-14-12-10-8-7-9-11-13-

InchiKey: LMXJIWNPDHVCFW-UHFFFAOYSA-N

Formula: C19H35ClO4

SMILES: CCC(CC)(C(=O)OCCCCCCCCCCl)C(=O)OCC(C)C

Mol. weight [g/mol]: 362.93

Physical Properties

Property code	Value	Unit	Source
gf	-370.27	kJ/mol	Joback Method
hf	-954.86	kJ/mol	Joback Method
hfus	43.80	kJ/mol	Joback Method
hvap	78.90	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	5.115		Crippen Method
mcvol	305.690	ml/mol	McGowan Method
pc	1141.34	kPa	Joback Method
rinpol	2262.00		NIST Webbook
tb	820.46	K	Joback Method
tc	1011.44	K	Joback Method
tf	465.55	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.07	J/mol×K	820.46	Joback Method
cpg	959.09	J/mol×K	852.29	Joback Method
cpg	975.06	J/mol×K	884.12	Joback Method
cpg	990.02	J/mol×K	915.95	Joback Method
cpg	1003.99	J/mol×K	947.78	Joback Method
cpg	1017.01	J/mol×K	979.61	Joback Method
cpg	1029.12	J/mol×K	1011.44	Joback Method
dvisc	0.0008193	Pa×s	465.55	Joback Method
dvisc	0.0003697	Pa×s	524.70	Joback Method

dvisc	0.0001961	Pa×s	583.85	Joback Method
dvisc	0.0001168	Pa×s	643.00	Joback Method
dvisc	0.0000760	Pa×s	702.16	Joback Method
dvisc	0.0000528	Pa×s	761.31	Joback Method
dvisc	0.0000387	Pa×s	820.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370750&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