Diethylmalonic acid, monochloride, 8-chlorooctyl ester

Inchi: InChI=1S/C15H26Cl2O3/c1-3-15(4-2,13(17)18)14(19)20-12-10-8-6-5-7-9-11-16/h3-12H2

InchiKey: CNVCGVRDINAEJD-UHFFFAOYSA-N

Formula: C15H26Cl2O3

SMILES: CCC(CC)(C(=O)Cl)C(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 325.27

Physical Properties

Property code	Value	Unit	Source
gf	-308.44	kJ/mol	Joback Method
hf	-750.54	kJ/mol	Joback Method
hfus	39.97	kJ/mol	Joback Method
hvap	72.36	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.681		Crippen Method
mcvol	255.700	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	2071.00		NIST Webbook
rinpol	2071.00		NIST Webbook
tb	744.39	K	Joback Method
tc	935.35	K	Joback Method
tf	443.16	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.91	J/mol×K	744.39	Joback Method
cpg	725.76	J/mol×K	776.22	Joback Method
cpg	739.74	J/mol×K	808.04	Joback Method
cpg	752.89	J/mol×K	839.87	Joback Method
cpg	765.25	J/mol×K	871.70	Joback Method
cpg	776.85	J/mol×K	903.53	Joback Method
cpg	787.73	J/mol×K	935.35	Joback Method
dvisc	0.0012784	Pa×s	443.16	Joback Method

dvisc	0.0006537	Pa×s	493.36	Joback Method
dvisc	0.0003784	Pa×s	543.57	Joback Method
dvisc	0.0002403	Pa×s	593.77	Joback Method
dvisc	0.0001637	Pa×s	643.98	Joback Method
dvisc	0.0001180	Pa×s	694.18	Joback Method
dvisc	0.0000888	Pa×s	744.39	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=U370759&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