Diethylmalonic acid, di(8-chlorooctyl) ester

Inchi: InChI=1S/C23H42Cl2O4/c1-3-23(4-2,21(26)28-19-15-11-7-5-9-13-17-24)22(27)29-20-16
InchiKey: FMHWGGNEXKANLA-UHFFFAOYSA-N
Formula: C23H42Cl2O4
SMILES: CCC(CC)(C(=O)OCCCCCCCCCl)C(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 453.48

Physical Properties

Property code	Value	Unit	Source
gf	-346.08	kJ/mol	Joback Method
hf	-1047.88	kJ/mol	Joback Method
hfus	61.88	kJ/mol	Joback Method
hvap	92.58	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	7.038		Crippen Method
mcvol	374.290	ml/mol	McGowan Method
pc	870.68	kPa	Joback Method
rinpol	2996.00		NIST Webbook
tb	949.85	K	Joback Method
tc	1163.65	K	Joback Method
tf	555.55	K	Joback Method
vc	1.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1214.66	J/mol×K	949.85	Joback Method
cpg	1232.20	J/mol×K	985.48	Joback Method
cpg	1248.43	J/mol×K	1021.12	Joback Method
cpg	1263.41	J/mol×K	1056.75	Joback Method
cpg	1277.21	J/mol×K	1092.38	Joback Method
cpg	1289.87	J/mol×K	1128.02	Joback Method
cpg	1301.47	J/mol×K	1163.65	Joback Method
dvisc	0.0003142	Pa×s	555.55	Joback Method
dvisc	0.0001525	Pa×s	621.27	Joback Method

dvisc	0.0000850	Pa×s	686.98	Joback Method
dvisc	0.0000525	Pa×s	752.70	Joback Method
dvisc	0.0000350	Pa×s	818.42	Joback Method
dvisc	0.0000248	Pa×s	884.13	Joback Method
dvisc	0.0000184	Pa×s	949.85	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=U370758&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