Diethylmalonic acid, 8-chlorooctyl octyl ester

Inchi: InChI=1S/C23H43ClO4/c1-4-7-8-9-13-16-19-27-21(25)23(5-2,6-3)22(26)28-20-17-14-11-
InchiKey: JMBOAYCMTXCVOU-UHFFFAOYSA-N
Formula: C23H43ClO4
SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 419.04

Physical Properties

Property code	Value	Unit	Source
gf	-334.15	kJ/mol	Joback Method
hf	-1032.14	kJ/mol	Joback Method
hfus	57.68	kJ/mol	Joback Method
hvap	88.19	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.819		Crippen Method
mcvol	362.050	ml/mol	McGowan Method
pc	890.00	kPa	Joback Method
rinpol	2660.00		NIST Webbook
rinpol	2660.00		NIST Webbook
tb	912.42	K	Joback Method
tc	1117.14	K	Joback Method
tf	525.63	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1185.82	J/mol×K	912.42	Joback Method
cpg	1204.30	J/mol×K	946.54	Joback Method
cpg	1221.50	J/mol×K	980.66	Joback Method
cpg	1237.47	J/mol×K	1014.78	Joback Method
cpg	1252.27	J/mol×K	1048.90	Joback Method
cpg	1265.96	J/mol×K	1083.02	Joback Method
cpg	1278.57	J/mol×K	1117.14	Joback Method
dvisc	0.0004149	Pa×s	525.63	Joback Method

dvisc	0.0001953	Pa×s	590.10	Joback Method
dvisc	0.0001067	Pa×s	654.56	Joback Method
dvisc	0.0000649	Pa×s	719.02	Joback Method
dvisc	0.0000429	Pa×s	783.49	Joback Method
dvisc	0.0000302	Pa×s	847.95	Joback Method
dvisc	0.0000223	Pa×s	912.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370754&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