Diethylmalonic acid, 8-chlorooctyl propyl ester

Inchi: InChI=1S/C18H33ClO4/c1-4-14-22-16(20)18(5-2,6-3)17(21)23-15-12-10-8-7-9-11-13-19/
InchiKey: JBZYMIOIVGRDCQ-UHFFFAOYSA-N
Formula: C18H33ClO4
SMILES: CCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 348.90

Physical Properties

Property code	Value	Unit	Source
gf	-376.25	kJ/mol	Joback Method
hf	-928.94	kJ/mol	Joback Method
hfus	44.73	kJ/mol	Joback Method
hvap	77.06	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.869		Crippen Method
mcvol	291.600	ml/mol	McGowan Method
pc	1212.36	kPa	Joback Method
rinpol	2217.00		NIST Webbook
tb	798.02	K	Joback Method
tc	986.05	K	Joback Method
tf	469.28	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.37	J/mol×K	798.02	Joback Method
cpg	898.95	J/mol×K	829.36	Joback Method
cpg	914.54	J/mol×K	860.70	Joback Method
cpg	929.19	J/mol×K	892.04	Joback Method
cpg	942.91	J/mol×K	923.38	Joback Method
cpg	955.73	J/mol×K	954.71	Joback Method
cpg	967.69	J/mol×K	986.05	Joback Method
dvisc	0.0007842	Pa×s	469.28	Joback Method
dvisc	0.0003884	Pa×s	524.07	Joback Method

dvisc	0.0002198	Pa×s	578.86	Joback Method
dvisc	0.0001372	Pa×s	633.65	Joback Method
dvisc	0.0000923	Pa×s	688.44	Joback Method
dvisc	0.0000659	Pa×s	743.23	Joback Method
dvisc	0.0000492	Pa×s	798.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370749&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