Diethylmalonic acid, 8-chlorooctyl pentyl ester

Inchi: InChI=1S/C20H37ClO4/c1-4-7-13-16-24-18(22)20(5-2,6-3)19(23)25-17-14-11-9-8-10-12-
InchiKey: SZGPZAZYCSKSGJ-UHFFFAOYSA-N
Formula: C20H37ClO4
SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 376.96

Physical Properties

Property code	Value	Unit	Source
gf	-359.41	kJ/mol	Joback Method
hf	-970.22	kJ/mol	Joback Method
hfus	49.91	kJ/mol	Joback Method
hvap	81.52	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.649		Crippen Method
mcvol	319.780	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	2389.00		NIST Webbook
rinpol	2389.00		NIST Webbook
tb	843.78	K	Joback Method
tc	1036.04	K	Joback Method
tf	491.82	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.58	J/mol×K	843.78	Joback Method
cpg	1077.52	J/mol×K	1004.00	Joback Method
cpg	1064.34	J/mol×K	971.96	Joback Method
cpg	1050.19	J/mol×K	939.91	Joback Method
cpg	1035.04	J/mol×K	907.87	Joback Method
cpg	1018.85	J/mol×K	875.82	Joback Method
cpg	1089.76	J/mol×K	1036.04	Joback Method
dvisc	0.0000360	Pa×s	843.78	Joback Method

dvisc	0.0000484	Pa×s	785.12	Joback Method
dvisc	0.0000683	Pa×s	726.46	Joback Method
dvisc	0.0001023	Pa×s	667.80	Joback Method
dvisc	0.0001657	Pa×s	609.14	Joback Method
dvisc	0.0002973	Pa×s	550.48	Joback Method
dvisc	0.0006134	Pa×s	491.82	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=U370751&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