Diethylmalonic acid, 8-chlorooctyl heptyl ester

Inchi: InChI=1S/C22H41ClO4/c1-4-7-8-12-15-18-26-20(24)22(5-2,6-3)21(25)27-19-16-13-10-9-
InchiKey: VUJOTVLZAGTTDX-UHFFFAOYSA-N
Formula: C22H41ClO4
SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 405.01

Physical Properties

Property code	Value	Unit	Source
gf	-342.57	kJ/mol	Joback Method
hf	-1011.50	kJ/mol	Joback Method
hfus	55.09	kJ/mol	Joback Method
hvap	85.97	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	6.429		Crippen Method
mcvol	347.960	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook
tb	889.54	K	Joback Method
tc	1089.21	K	Joback Method
tf	514.36	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1123.76	J/mol×K	889.54	Joback Method
cpg	1202.42	J/mol×K	1055.93	Joback Method
cpg	1188.91	J/mol×K	1022.65	Joback Method
cpg	1174.33	J/mol×K	989.37	Joback Method
cpg	1158.65	J/mol×K	956.10	Joback Method
cpg	1141.80	J/mol×K	922.82	Joback Method
cpg	1214.92	J/mol×K	1089.21	Joback Method
dvisc	0.0000262	Pa×s	889.54	Joback Method

dvisc	0.0000354	Pa×s	827.01	Joback Method
dvisc	0.0000502	Pa×s	764.48	Joback Method
dvisc	0.0000757	Pa×s	701.95	Joback Method
dvisc	0.0001238	Pa×s	639.42	Joback Method
dvisc	0.0002252	Pa×s	576.89	Joback Method
dvisc	0.0004739	Pa×s	514.36	Joback Method

Sources

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=U370753&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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