Diethylmalonic acid, 8-chlorooctyl decyl ester

Inchi: InChI=1S/C25H47ClO4/c1-4-7-8-9-10-12-15-18-21-29-23(27)25(5-2,6-3)24(28)30-22-19-
InchiKey: ORBFXPQCSJDJPN-UHFFFAOYSA-N
Formula: C25H47ClO4
SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 447.09

Physical Properties

Property code	Value	Unit	Source
gf	-317.31	kJ/mol	Joback Method
hf	-1073.42	kJ/mol	Joback Method
hfus	62.86	kJ/mol	Joback Method
hvap	92.64	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	7.599		Crippen Method
mcvol	390.230	ml/mol	McGowan Method
pc	796.18	kPa	Joback Method
rinpol	2849.00		NIST Webbook
rinpol	2849.00		NIST Webbook
tb	958.18	K	Joback Method
tc	1176.09	K	Joback Method
tf	548.17	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1311.59	J/mol×K	958.18	Joback Method
cpg	1395.01	J/mol×K	1139.77	Joback Method
cpg	1380.97	J/mol×K	1103.45	Joback Method
cpg	1365.68	J/mol×K	1067.13	Joback Method
cpg	1349.07	J/mol×K	1030.82	Joback Method
cpg	1331.06	J/mol×K	994.50	Joback Method
cpg	1407.86	J/mol×K	1176.09	Joback Method
dvisc	0.0000161	Pa×s	958.18	Joback Method

dvisc	0.0000218	Pa×s	889.85	Joback Method
dvisc	0.0000312	Pa×s	821.51	Joback Method
dvisc	0.0000475	Pa×s	753.17	Joback Method
dvisc	0.0000788	Pa×s	684.84	Joback Method
dvisc	0.0001460	Pa×s	616.51	Joback Method
dvisc	0.0003157	Pa×s	548.17	Joback Method

Sources

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=U370756&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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