Diethylmalonic acid, 8-chlorooctyl hexyl ester

Inchi: InChI=1S/C21H39ClO4/c1-4-7-8-14-17-25-19(23)21(5-2,6-3)20(24)26-18-15-12-10-9-11-
InchiKey: BJGQOOJGGDOVGA-UHFFFAOYSA-N
Formula: C21H39ClO4
SMILES: CCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 390.99

Physical Properties

Property code	Value	Unit	Source
gf	-350.99	kJ/mol	Joback Method
hf	-990.86	kJ/mol	Joback Method
hfus	52.50	kJ/mol	Joback Method
hvap	83.74	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	6.039		Crippen Method
mcvol	333.870	ml/mol	McGowan Method
pc	1001.44	kPa	Joback Method
rinpol	2479.00		NIST Webbook
tb	866.66	K	Joback Method
tc	1062.20	K	Joback Method
tf	503.09	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.33	J/mol×K	866.66	Joback Method
cpg	1079.97	J/mol×K	899.25	Joback Method
cpg	1096.48	J/mol×K	931.84	Joback Method
cpg	1111.89	J/mol×K	964.43	Joback Method
cpg	1126.25	J/mol×K	997.02	Joback Method
cpg	1139.60	J/mol×K	1029.61	Joback Method
cpg	1151.97	J/mol×K	1062.20	Joback Method
dvisc	0.0005399	Pa×s	503.09	Joback Method
dvisc	0.0002591	Pa×s	563.69	Joback Method

dvisc	0.0001434	Pa×s	624.28	Joback Method
dvisc	0.0000881	Pa×s	684.88	Joback Method
dvisc	0.0000586	Pa×s	745.47	Joback Method
dvisc	0.0000414	Pa×s	806.07	Joback Method
dvisc	0.0000308	Pa×s	866.66	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=U370752&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

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