Diethylmalonic acid, monochloride, hexadecyl ester

Inchi: InChI=1S/C23H43ClO3/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-27-22(26)23(5-2,6

InchiKey: RPVMNBGMWRQOID-UHFFFAOYSA-N

Formula: C23H43ClO3

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Cl

Mol. weight [g/mol]: 403.04

Physical Properties

Property code	Value	Unit	Source
gf	-229.15	kJ/mol	Joback Method
hf	-899.92	kJ/mol	Joback Method
hfus	56.49	kJ/mol	Joback Method
hvap	85.78	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	7.583		Crippen Method
mcvol	356.180	ml/mol	McGowan Method
pc	899.10	kPa	Joback Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	890.00	K	Joback Method
tc	1089.72	K	Joback Method
tf	503.40	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1154.42	J/mol×K	890.00	Joback Method
cpg	1237.38	J/mol×K	1056.43	Joback Method
cpg	1222.86	J/mol×K	1023.14	Joback Method
cpg	1207.37	J/mol×K	989.86	Joback Method
cpg	1190.84	J/mol×K	956.57	Joback Method
cpg	1173.21	J/mol×K	923.29	Joback Method
cpg	1250.99	J/mol×K	1089.72	Joback Method
dvisc	0.0000304	Pa×s	890.00	Joback Method

dvisc	0.0000413	Pa×s	825.57	Joback Method
dvisc	0.0000592	Pa×s	761.13	Joback Method
dvisc	0.0000906	Pa×s	696.70	Joback Method
dvisc	0.0001513	Pa×s	632.27	Joback Method
dvisc	0.0002836	Pa×s	567.83	Joback Method
dvisc	0.0006246	Pa×s	503.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369725&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