Diethylmalonic acid, 2-chloro-5-methylphenyl hexyl ester

Inchi: InChI=1S/C20H29ClO4/c1-5-8-9-10-13-24-18(22)20(6-2,7-3)19(23)25-17-14-15(4)11-12-

InchiKey: CQVSVHKRAKLENJ-UHFFFAOYSA-N

Formula: C20H29ClO4

SMILES: CCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 368.89

Physical Properties

Property code	Value	Unit	Source
gf	-266.26	kJ/mol	Joback Method
hf	-756.63	kJ/mol	Joback Method
hfus	43.18	kJ/mol	Joback Method
hvap	85.11	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.484		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1309.90	kPa	Joback Method
rinpol	2338.00		NIST Webbook
rinpol	2338.00		NIST Webbook
tb	880.42	K	Joback Method
tc	1091.11	K	Joback Method
tf	543.28	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.87	J/mol×K	880.42	Joback Method
cpg	919.87	J/mol×K	915.53	Joback Method
cpg	933.72	J/mol×K	950.65	Joback Method
cpg	946.46	J/mol×K	985.76	Joback Method
cpg	958.13	J/mol×K	1020.88	Joback Method
cpg	968.77	J/mol×K	1055.99	Joback Method
cpg	978.42	J/mol×K	1091.11	Joback Method
dvisc	0.0003763	Pa×s	543.28	Joback Method

dvisc	0.0002140	Pa×s	599.47	Joback Method
dvisc	0.0001340	Pa×s	655.66	Joback Method
dvisc	0.0000904	Pa×s	711.85	Joback Method
dvisc	0.0000646	Pa×s	768.04	Joback Method
dvisc	0.0000483	Pa×s	824.23	Joback Method
dvisc	0.0000375	Pa×s	880.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370456&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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