Dimethylmalonic acid, dodecyl pentachlorophenyl ester

Inchi: InChI=1S/C23H31Cl5O4/c1-4-5-6-7-8-9-10-11-12-13-14-31-21(29)23(2,3)22(30)32-20-18

InchiKey: OIXATLVZKLVBLC-UHFFFAOYSA-N

Formula: C23H31Cl5O4

SMILES: CCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 548.75

Physical Properties

Property code	Value	Unit	Source
gf	-317.61	kJ/mol	Joback Method
hf	-915.92	kJ/mol	Joback Method
hfus	66.57	kJ/mol	Joback Method
hvap	111.32	kJ/mol	Joback Method
log10ws	-10.11		Crippen Method
logp	9.349		Crippen Method
mcvol	387.250	ml/mol	McGowan Method
pc	950.25	kPa	Joback Method
rinpol	3444.00		NIST Webbook
rinpol	3444.00		NIST Webbook
tb	1113.72	K	Joback Method
tc	1364.34	K	Joback Method
tf	734.33	K	Joback Method
vc	1.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1166.42	J/mol×K	1113.72	Joback Method
cpg	1205.40	J/mol×K	1322.57	Joback Method
cpg	1200.19	J/mol×K	1280.80	Joback Method
cpg	1193.75	J/mol×K	1239.03	Joback Method
cpg	1186.02	J/mol×K	1197.26	Joback Method
cpg	1176.94	J/mol×K	1155.49	Joback Method
cpg	1209.46	J/mol×K	1364.34	Joback Method
dvisc	0.0000120	Pa×s	1113.72	Joback Method

dvisc	0.0000149	Pa×s	1050.49	Joback Method
dvisc	0.0000191	Pa×s	987.26	Joback Method
dvisc	0.0000254	Pa×s	924.02	Joback Method
dvisc	0.0000352	Pa×s	860.79	Joback Method
dvisc	0.0000512	Pa×s	797.56	Joback Method
dvisc	0.0000797	Pa×s	734.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363932&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