Dimethylmalonic acid, ethyl pentachlorophenyl ester

Inchi: InChI=1S/C13H11Cl5O4/c1-4-21-11(19)13(2,3)12(20)22-10-8(17)6(15)5(14)7(16)9(10)18

InchiKey: BUDYUENCDUJLKS-UHFFFAOYSA-N

Formula: C13H11Cl5O4

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

Mol. weight [g/mol]: 408.49

Physical Properties

Property code	Value	Unit	Source
gf	-401.81	kJ/mol	Joback Method
hf	-709.52	kJ/mol	Joback Method
hfus	40.67	kJ/mol	Joback Method
hvap	89.06	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.448		Crippen Method
mcvol	246.350	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2462.00		NIST Webbook
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tb	884.92	K	Joback Method
tc	1121.55	K	Joback Method
tf	621.63	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.56	J/mol×K	884.92	Joback Method
cpg	600.85	J/mol×K	924.36	Joback Method
cpg	608.20	J/mol×K	963.80	Joback Method
cpg	614.63	J/mol×K	1003.23	Joback Method
cpg	620.16	J/mol×K	1042.67	Joback Method
cpg	624.78	J/mol×K	1082.11	Joback Method
cpg	628.53	J/mol×K	1121.55	Joback Method
dvisc	0.0002616	Pa×s	621.63	Joback Method

dvisc	0.0001874	Pa×s	665.51	Joback Method
dvisc	0.0001399	Pa×s	709.39	Joback Method
dvisc	0.0001080	Pa×s	753.27	Joback Method
dvisc	0.0000859	Pa×s	797.16	Joback Method
dvisc	0.0000699	Pa×s	841.04	Joback Method
dvisc	0.0000581	Pa×s	884.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363926&Units=SI

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