Dimethylmalonic acid, pentachlorophenyl pentyl ester

Inchi: InChI=1S/C16H17Cl5O4/c1-4-5-6-7-24-14(22)16(2,3)15(23)25-13-11(20)9(18)8(17)10(19

InchiKey: NEPNDOICGJFDPC-UHFFFAOYSA-N

Formula: C16H17Cl5O4

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

Mol. weight [g/mol]: 450.57

Physical Properties

Property code	Value	Unit	Source
gf	-376.55	kJ/mol	Joback Method
hf	-771.44	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	95.74	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.619		Crippen Method
mcvol	288.620	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	2735.00		NIST Webbook
rinpol	2735.00		NIST Webbook
tb	953.56	K	Joback Method
tc	1184.98	K	Joback Method
tf	655.44	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.98	J/mol×K	953.56	Joback Method
cpg	767.17	J/mol×K	992.13	Joback Method
cpg	775.31	J/mol×K	1030.70	Joback Method
cpg	782.44	J/mol×K	1069.27	Joback Method
cpg	788.58	J/mol×K	1107.84	Joback Method
cpg	793.74	J/mol×K	1146.41	Joback Method
cpg	797.95	J/mol×K	1184.98	Joback Method
dvisc	0.0001883	Pa×s	655.44	Joback Method

dvisc	0.0001302	Pa×s	705.13	Joback Method
dvisc	0.0000946	Pa×s	754.81	Joback Method
dvisc	0.0000714	Pa×s	804.50	Joback Method
dvisc	0.0000558	Pa×s	854.19	Joback Method
dvisc	0.0000447	Pa×s	903.87	Joback Method
dvisc	0.0000367	Pa×s	953.56	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=U363927&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