Dimethylmalonic acid, hexyl pentachlorophenyl ester

Inchi: InChI=1S/C17H19Cl5O4/c1-4-5-6-7-8-25-15(23)17(2,3)16(24)26-14-12(21)10(19)9(18)11

InchiKey: JBSWAYORSIHUHR-UHFFFAOYSA-N

Formula: C17H19Cl5O4

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

Mol. weight [g/mol]: 464.60

Physical Properties

Property code	Value	Unit	Source
gf	-368.13	kJ/mol	Joback Method
hf	-792.08	kJ/mol	Joback Method
hfus	51.03	kJ/mol	Joback Method
hvap	97.96	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	7.009		Crippen Method
mcvol	302.710	ml/mol	McGowan Method
pc	1404.84	kPa	Joback Method
rinpol	2833.00		NIST Webbook
rinpol	2833.00		NIST Webbook
tb	976.44	K	Joback Method
tc	1207.71	K	Joback Method
tf	666.71	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.62	J/mol×K	976.44	Joback Method
cpg	851.16	J/mol×K	1169.16	Joback Method
cpg	845.90	J/mol×K	1130.62	Joback Method
cpg	839.65	J/mol×K	1092.07	Joback Method
cpg	832.37	J/mol×K	1053.53	Joback Method
cpg	824.03	J/mol×K	1014.98	Joback Method
cpg	855.44	J/mol×K	1207.71	Joback Method
dvisc	0.0000314	Pa×s	976.44	Joback Method

dvisc	0.0000384	Pa×s	924.82	Joback Method
dvisc	0.0000481	Pa×s	873.20	Joback Method
dvisc	0.0000620	Pa×s	821.57	Joback Method
dvisc	0.0000826	Pa×s	769.95	Joback Method
dvisc	0.0001147	Pa×s	718.33	Joback Method
dvisc	0.0001677	Pa×s	666.71	Joback Method

Sources

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=U363929&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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