Dimethylmalonic acid, dipentafluorophenyl ester

Inchi: InChI=1S/C17H6F10O4/c1-17(2,15(28)30-13-9(24)5(20)3(18)6(21)10(13)25)16(29)31-14
InchiKey: WWFPQFWWTZIEIC-UHFFFAOYSA-N
Formula: C17H6F10O4
SMILES: CC(C)(C(=O)Oc1c(F)c(F)c(F)c(F)c1F)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 464.21

Physical Properties

Property code	Value	Unit	Source
gf	-2192.32	kJ/mol	Joback Method
hf	-2495.30	kJ/mol	Joback Method
hfus	52.94	kJ/mol	Joback Method
hvap	73.45	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	4.615		Crippen Method
mcvol	235.450	ml/mol	McGowan Method
pc	1395.41	kPa	Joback Method
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
tb	833.57	K	Joback Method
tc	1024.37	K	Joback Method
tf	612.03	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.31	J/mol×K	833.57	Joback Method
cpg	686.39	J/mol×K	865.37	Joback Method
cpg	694.68	J/mol×K	897.17	Joback Method
cpg	702.19	J/mol×K	928.97	Joback Method
cpg	708.92	J/mol×K	960.77	Joback Method
cpg	714.86	J/mol×K	992.57	Joback Method
cpg	720.01	J/mol×K	1024.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363676&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

Legend

cpg:	Ideal gas heat capacity
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