Dimethylmalonic acid, hexyl pentafluorophenyl ester

Inchi: InChI=1S/C17H19F5O4/c1-4-5-6-7-8-25-15(23)17(2,3)16(24)26-14-12(21)10(19)9(18)11

InchiKey: DDVIMLOIAVWIRB-UHFFFAOYSA-N

Formula: C17H19F5O4

SMILES: CCCCCCOC(=O)C(C)(C)C(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 382.32

Physical Properties

Property code	Value	Unit	Source
gf	-1282.53	kJ/mol	Joback Method
hf	-1693.93	kJ/mol	Joback Method
hfus	45.44	kJ/mol	Joback Method
hvap	71.95	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.437		Crippen Method
mcvol	250.360	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1753.00		NIST Webbook
rinpol	1753.00		NIST Webbook
tb	785.64	K	Joback Method
tc	971.07	K	Joback Method
tf	520.06	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.90	J/mol×K	785.64	Joback Method
cpg	753.91	J/mol×K	816.55	Joback Method
cpg	766.10	J/mol×K	847.45	Joback Method
cpg	777.47	J/mol×K	878.36	Joback Method
cpg	788.04	J/mol×K	909.26	Joback Method
cpg	797.81	J/mol×K	940.17	Joback Method
cpg	806.79	J/mol×K	971.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363663&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
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