Dimethylmalonic acid, isohexyl pentafluorophenyl ester

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

InchiKey: KRLAYCLHTKNNET-UHFFFAOYSA-N

Formula: C17H19F5O4

SMILES: CC(C)CCCOC(=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	-1284.97	kJ/mol	Joback Method
hf	-1699.21	kJ/mol	Joback Method
hfus	41.92	kJ/mol	Joback Method
hvap	71.56	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.293		Crippen Method
mcvol	250.360	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tb	785.20	K	Joback Method
tc	972.14	K	Joback Method
tf	505.06	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.46	J/mol×K	785.20	Joback Method
cpg	754.58	J/mol×K	816.36	Joback Method
cpg	766.86	J/mol×K	847.51	Joback Method
cpg	778.29	J/mol×K	878.67	Joback Method
cpg	788.90	J/mol×K	909.82	Joback Method
cpg	798.69	J/mol×K	940.98	Joback Method
cpg	807.68	J/mol×K	972.14	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=U363662&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
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