Dimethylmalonic acid, 2,2,3,4,4,4-hexafluorobutyl nonyl ester

Inchi: InChI=1S/C18H28F6O4/c1-4-5-6-7-8-9-10-11-27-14(25)16(2,3)15(26)28-12-17(20,21)13

InchiKey: MRADZBZJACRLEP-UHFFFAOYSA-N

Formula: C18H28F6O4

SMILES: CCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)C(F)(F)F

Mol. weight [g/mol]: 422.40

Physical Properties

Property code	Value	Unit	Source
gf	-1529.94	kJ/mol	Joback Method
hf	-2112.64	kJ/mol	Joback Method
hfus	40.66	kJ/mol	Joback Method
hvap	64.80	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.385		Crippen Method
mcvol	289.980	ml/mol	McGowan Method
pc	1068.66	kPa	Joback Method
rinpol	1716.00		NIST Webbook
tb	749.31	K	Joback Method
tc	921.08	K	Joback Method
tf	432.74	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.65	J/mol×K	749.31	Joback Method
cpg	916.32	J/mol×K	777.94	Joback Method
cpg	931.07	J/mol×K	806.57	Joback Method
cpg	944.96	J/mol×K	835.20	Joback Method
cpg	958.03	J/mol×K	863.82	Joback Method
cpg	970.33	J/mol×K	892.45	Joback Method
cpg	981.89	J/mol×K	921.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361993&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