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

Inchi: InChI=1S/C17H26F6O4/c1-4-5-6-7-8-9-10-26-13(24)15(2,3)14(25)27-11-16(19,20)12(18)17(21,22)23/h12H,4-11H2,1-3H3

InchiKey: XEEOWRVTLYJPCL-UHFFFAOYSA-N

Formula: C17H26F6O4

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

Mol. weight [g/mol]: 408.38

Physical Properties

Property code	Value	Unit	Source
gf	-1538.36	kJ/mol	Joback Method
hf	-2092.00	kJ/mol	Joback Method
hfus	38.07	kJ/mol	Joback Method
hvap	62.57	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.995		Crippen Method
mcvol	275.890	ml/mol	McGowan Method
pc	1139.03	kPa	Joback Method
rinpol	1624.00		NIST Webbook
rinpol	1624.00		NIST Webbook
tb	726.43	K	Joback Method
tc	895.74	K	Joback Method
tf	421.47	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.48	J/mol×K	726.43	Joback Method
cpg	858.72	J/mol×K	754.65	Joback Method
cpg	873.09	J/mol×K	782.87	Joback Method
cpg	886.62	J/mol×K	811.08	Joback Method
cpg	899.35	J/mol×K	839.30	Joback Method
cpg	911.33	J/mol×K	867.52	Joback Method
cpg	922.60	J/mol×K	895.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361992&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