Malonic acid, di(2,2,3,3,4,4,5,5-octafluoropentyl) ester

Inchi: InChI=1S/C13H8F16O4/c14-6(15)10(22,23)12(26,27)8(18,19)2-32-4(30)1-5(31)33-3-9(2(

InchiKey: DHLQIUYEPAFTHY-UHFFFAOYSA-N

Formula: C13H8F16O4

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

Mol. weight [g/mol]: 532.17

Physical Properties

Property code	Value	Unit	Source
gf	-3514.06	kJ/mol	Joback Method
hf	-4002.07	kJ/mol	Joback Method
hfus	32.75	kJ/mol	Joback Method
hvap	41.22	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.805		Crippen Method
mcvol	237.230	ml/mol	McGowan Method
pc	1138.27	kPa	Joback Method
rinpol	1292.00		NIST Webbook
rinpol	1292.00		NIST Webbook
tb	617.48	K	Joback Method
tc	759.97	K	Joback Method
tf	374.55	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.26	J/mol×K	617.48	Joback Method
cpg	726.64	J/mol×K	641.23	Joback Method
cpg	737.24	J/mol×K	664.98	Joback Method
cpg	747.09	J/mol×K	688.73	Joback Method
cpg	756.25	J/mol×K	712.48	Joback Method
cpg	764.76	J/mol×K	736.22	Joback Method
cpg	772.66	J/mol×K	759.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349355&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

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