Malonic acid, 2,2,3,3,4,4,5,5-octafluoropentyl pentyl ester

Inchi: InChI=1S/C13H16F8O4/c1-2-3-4-5-24-8(22)6-9(23)25-7-11(16,17)13(20,21)12(18,19)10(

InchiKey: WGDFIMFYQDLSPX-UHFFFAOYSA-N

Formula: C13H16F8O4

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

Mol. weight [g/mol]: 388.25

Physical Properties

Property code	Value	Unit	Source
gf	-1961.66	kJ/mol	Joback Method
hf	-2401.66	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	52.03	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.824		Crippen Method
mcvol	223.070	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	1465.00		NIST Webbook
rinpol	1465.00		NIST Webbook
tb	633.45	K	Joback Method
tc	789.46	K	Joback Method
tf	377.57	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.44	J/mol×K	633.45	Joback Method
cpg	654.22	J/mol×K	659.45	Joback Method
cpg	666.29	J/mol×K	685.45	Joback Method
cpg	677.68	J/mol×K	711.46	Joback Method
cpg	688.41	J/mol×K	737.46	Joback Method
cpg	698.51	J/mol×K	763.46	Joback Method
cpg	708.01	J/mol×K	789.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349349&Units=SI

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