Dimethylmalonic acid, di(2,2,3,4,4,4-hexafluorobutyl) ester

Inchi: InChI=1S/C13H12F12O4/c1-9(2,7(26)28-3-10(16,17)5(14)12(20,21)22)8(27)29-4-11(18,1

InchiKey: KNJMSYHWQPHIMV-UHFFFAOYSA-N

Formula: C13H12F12O4

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

Mol. weight [g/mol]: 460.21

Physical Properties

Property code	Value	Unit	Source
gf	-2737.66	kJ/mol	Joback Method
hf	-3208.88	kJ/mol	Joback Method
hfus	27.84	kJ/mol	Joback Method
hvap	45.78	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.170		Crippen Method
mcvol	230.150	ml/mol	McGowan Method
pc	1272.78	kPa	Joback Method
rinpol	1132.00		NIST Webbook
rinpol	1132.00		NIST Webbook
tb	623.63	K	Joback Method
tc	774.43	K	Joback Method
tf	369.77	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.99	J/mol×K	623.63	Joback Method
cpg	692.15	J/mol×K	648.76	Joback Method
cpg	703.53	J/mol×K	673.90	Joback Method
cpg	714.15	J/mol×K	699.03	Joback Method
cpg	724.06	J/mol×K	724.17	Joback Method
cpg	733.31	J/mol×K	749.30	Joback Method
cpg	741.94	J/mol×K	774.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361994&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