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

Inchi: InChI=1S/C16H24F6O4/c1-4-5-6-7-8-9-25-12(23)14(2,3)13(24)26-10-15(18,19)11(17)16

InchiKey: FSIAYMRFHHQRRY-UHFFFAOYSA-N

Formula: C16H24F6O4

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

Mol. weight [g/mol]: 394.35

Physical Properties

Property code	Value	Unit	Source
gf	-1546.78	kJ/mol	Joback Method
hf	-2071.36	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	60.34	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.605		Crippen Method
mcvol	261.800	ml/mol	McGowan Method
pc	1216.59	kPa	Joback Method
rinpol	1534.00		NIST Webbook
tb	703.55	K	Joback Method
tc	871.01	K	Joback Method
tf	410.20	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.30	J/mol×K	703.55	Joback Method
cpg	802.13	J/mol×K	731.46	Joback Method
cpg	816.11	J/mol×K	759.37	Joback Method
cpg	829.29	J/mol×K	787.28	Joback Method
cpg	841.69	J/mol×K	815.19	Joback Method
cpg	853.35	J/mol×K	843.10	Joback Method
cpg	864.33	J/mol×K	871.01	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=U361991&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