Dimethylmalonic acid, heptyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C15H23F5O4/c1-4-5-6-7-8-9-23-11(21)13(2,3)12(22)24-10-14(16,17)15(18,19)

InchiKey: YEQAAEYTYASDDY-UHFFFAOYSA-N

Formula: C15H23F5O4

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

Mol. weight [g/mol]: 362.33

Physical Properties

Property code	Value	Unit	Source
gf	-1357.95	kJ/mol	Joback Method
hf	-1849.33	kJ/mol	Joback Method
hfus	33.34	kJ/mol	Joback Method
hvap	59.32	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.267		Crippen Method
mcvol	245.940	ml/mol	McGowan Method
pc	1337.84	kPa	Joback Method
rinpol	1427.00		NIST Webbook
rinpol	1427.00		NIST Webbook
tb	681.84	K	Joback Method
tc	850.44	K	Joback Method
tf	413.34	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.82	J/mol×K	681.84	Joback Method
cpg	738.48	J/mol×K	709.94	Joback Method
cpg	752.30	J/mol×K	738.04	Joback Method
cpg	765.33	J/mol×K	766.14	Joback Method
cpg	777.60	J/mol×K	794.24	Joback Method
cpg	789.15	J/mol×K	822.34	Joback Method
cpg	800.03	J/mol×K	850.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361941&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