Diethylmalonic acid, isobutyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C14H21F5O4/c1-5-12(6-2,10(20)22-7-9(3)4)11(21)23-8-13(15,16)14(17,18)19/

InchiKey: GKGLJXZSBCVIML-UHFFFAOYSA-N

Formula: C14H21F5O4

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

Mol. weight [g/mol]: 348.31

Physical Properties

Property code	Value	Unit	Source
gf	-1368.81	kJ/mol	Joback Method
hf	-1833.97	kJ/mol	Joback Method
hfus	27.22	kJ/mol	Joback Method
hvap	56.71	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.733		Crippen Method
mcvol	231.850	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
rinpol	1237.00		NIST Webbook
rinpol	1237.00		NIST Webbook
tb	658.52	K	Joback Method
tc	828.71	K	Joback Method
tf	387.07	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.23	J/mol×K	658.52	Joback Method
cpg	684.69	J/mol×K	686.88	Joback Method
cpg	698.32	J/mol×K	715.25	Joback Method
cpg	711.14	J/mol×K	743.61	Joback Method
cpg	723.21	J/mol×K	771.98	Joback Method
cpg	734.54	J/mol×K	800.34	Joback Method
cpg	745.19	J/mol×K	828.71	Joback Method

Sources

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=U370839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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