Diethylmalonic acid, isobutyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C14H23F3O4/c1-6-13(7-2,11(18)20-8-9(3)4)12(19)21-10(5)14(15,16)17/h9-10H

InchiKey: CAPXWQRHMYIMDV-UHFFFAOYSA-N

Formula: C14H23F3O4

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

Mol. weight [g/mol]: 312.33

Physical Properties

Property code	Value	Unit	Source
gf	-984.47	kJ/mol	Joback Method
hf	-1438.28	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	59.25	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.486		Crippen Method
mcvol	228.310	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	1295.00		NIST Webbook
rinpol	1295.00		NIST Webbook
tb	662.77	K	Joback Method
tc	839.82	K	Joback Method
tf	368.47	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.09	J/mol×K	662.77	Joback Method
cpg	667.41	J/mol×K	692.28	Joback Method
cpg	681.88	J/mol×K	721.79	Joback Method
cpg	695.52	J/mol×K	751.29	Joback Method
cpg	708.38	J/mol×K	780.80	Joback Method
cpg	720.46	J/mol×K	810.31	Joback Method
cpg	731.82	J/mol×K	839.82	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=U370815&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