Diethylmalonic acid, isobutyl 2-fluoroethyl ester

Inchi: InChI=1S/C13H23FO4/c1-5-13(6-2,11(15)17-8-7-14)12(16)18-9-10(3)4/h10H,5-9H2,1-4H

InchiKey: DBQMANTWSJRXEX-UHFFFAOYSA-N

Formula: C13H23FO4

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

Mol. weight [g/mol]: 262.32

Physical Properties

Property code	Value	Unit	Source
gf	-603.67	kJ/mol	Joback Method
hf	-1011.39	kJ/mol	Joback Method
hfus	27.14	kJ/mol	Joback Method
hvap	60.34	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.505		Crippen Method
mcvol	210.680	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	1419.00		NIST Webbook
tb	645.02	K	Joback Method
tc	825.32	K	Joback Method
tf	368.60	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.61	J/mol×K	645.02	Joback Method
cpg	594.90	J/mol×K	675.07	Joback Method
cpg	609.42	J/mol×K	705.12	Joback Method
cpg	623.19	J/mol×K	735.17	Joback Method
cpg	636.21	J/mol×K	765.22	Joback Method
cpg	648.51	J/mol×K	795.27	Joback Method
cpg	660.09	J/mol×K	825.32	Joback Method

Sources

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=U370858&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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