Diethylmalonic acid, di(2-fluoroethyl) ester

Inchi: InChI=1S/C11H18F2O4/c1-3-11(4-2,9(14)16-7-5-12)10(15)17-8-6-13/h3-8H2,1-2H3
InchiKey: DYHDLDQOKLCONU-UHFFFAOYSA-N
Formula: C11H18F2O4
SMILES: CCC(CC)(C(=O)OCCF)C(=O)OCCF
Mol. weight [g/mol]: 252.25

Physical Properties

Property code	Value	Unit	Source
gf	-812.88	kJ/mol	Joback Method
hf	-1160.94	kJ/mol	Joback Method
hfus	28.57	kJ/mol	Joback Method
hvap	55.46	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.818		Crippen Method
mcvol	184.270	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1345.00		NIST Webbook
tb	598.97	K	Joback Method
tc	772.03	K	Joback Method
tf	361.65	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.43	J/mol×K	598.97	Joback Method
cpg	497.78	J/mol×K	627.81	Joback Method
cpg	510.51	J/mol×K	656.66	Joback Method
cpg	522.61	J/mol×K	685.50	Joback Method
cpg	534.11	J/mol×K	714.34	Joback Method
cpg	545.01	J/mol×K	743.18	Joback Method
cpg	555.32	J/mol×K	772.03	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=U370868&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