Diethylmalonic acid, 2-fluoroethyl pentyl ester

Inchi: InChI=1S/C14H25FO4/c1-4-7-8-10-18-12(16)14(5-2,6-3)13(17)19-11-9-15/h4-11H2,1-3H
InchiKey: JVJPIZULWPTJPE-UHFFFAOYSA-N
Formula: C14H25FO4
SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)OCCF
Mol. weight [g/mol]: 276.34

Physical Properties

Property code	Value	Unit	Source
gf	-592.81	kJ/mol	Joback Method
hf	-1026.75	kJ/mol	Joback Method
hfus	33.26	kJ/mol	Joback Method
hvap	62.96	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.039		Crippen Method
mcvol	224.770	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
tb	668.34	K	Joback Method
tc	845.26	K	Joback Method
tf	394.87	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.68	J/mol×K	668.34	Joback Method
cpg	648.18	J/mol×K	697.83	Joback Method
cpg	662.91	J/mol×K	727.31	Joback Method
cpg	676.87	J/mol×K	756.80	Joback Method
cpg	690.09	J/mol×K	786.29	Joback Method
cpg	702.59	J/mol×K	815.77	Joback Method
cpg	714.37	J/mol×K	845.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370860&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