Glutaric acid, hept-2-yl 2-fluoroethyl ester

Inchi: InChI=1S/C14H25FO4/c1-3-4-5-7-12(2)19-14(17)9-6-8-13(16)18-11-10-15/h12H,3-11H2
InchiKey: YJKAHJNOPXPSHO-UHFFFAOYSA-N
Formula: C14H25FO4
SMILES: CCCCCC(C)OC(=O)CCCC(=O)OCCF
Mol. weight [g/mol]: 276.34

Physical Properties

Property code	Value	Unit	Source
gf	-598.09	kJ/mol	Joback Method
hf	-1023.28	kJ/mol	Joback Method
hfus	37.15	kJ/mol	Joback Method
hvap	63.86	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.181		Crippen Method
mcvol	224.770	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	1702.00		NIST Webbook
rinpol	1702.00		NIST Webbook
tb	671.13	K	Joback Method
tc	844.01	K	Joback Method
tf	377.45	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.55	J/mol×K	671.13	Joback Method
cpg	645.89	J/mol×K	699.94	Joback Method
cpg	660.53	J/mol×K	728.76	Joback Method
cpg	674.46	J/mol×K	757.57	Joback Method
cpg	687.68	J/mol×K	786.38	Joback Method
cpg	700.20	J/mol×K	815.20	Joback Method
cpg	712.04	J/mol×K	844.01	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=U393710&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