Glutaric acid, hex-4-yn-3-yl 2-fluoroethyl ester

Inchi: InChI=1S/C13H19FO4/c1-3-6-11(4-2)18-13(16)8-5-7-12(15)17-10-9-14/h11H,4-5,7-10H2
InchiKey: BECHCUNYJRPELH-UHFFFAOYSA-N
Formula: C13H19FO4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCCF
Mol. weight [g/mol]: 258.29

Physical Properties

Property code	Value	Unit	Source
gf	-403.71	kJ/mol	Joback Method
hf	-730.34	kJ/mol	Joback Method
hfus	37.68	kJ/mol	Joback Method
hvap	63.79	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.014		Crippen Method
mcvol	202.080	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	1671.00		NIST Webbook
rinpol	1671.00		NIST Webbook
tb	657.25	K	Joback Method
tc	846.01	K	Joback Method
tf	472.28	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.43	J/mol×K	657.25	Joback Method
cpg	548.62	J/mol×K	688.71	Joback Method
cpg	562.12	J/mol×K	720.17	Joback Method
cpg	574.92	J/mol×K	751.63	Joback Method
cpg	587.02	J/mol×K	783.09	Joback Method
cpg	598.43	J/mol×K	814.55	Joback Method
cpg	609.14	J/mol×K	846.01	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=U393709&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