Glutaric acid, 2-methylpent-3-yl 2-fluoroethyl ester

Inchi: InChI=1S/C13H23FO4/c1-4-11(10(2)3)18-13(16)7-5-6-12(15)17-9-8-14/h10-11H,4-9H2,1

InchiKey: LAGOXVCCDCKUSW-UHFFFAOYSA-N

Formula: C13H23FO4

SMILES: CCC(OC(=O)CCCC(=O)OCCF)C(C)C

Mol. weight [g/mol]: 262.32

Physical Properties

Property code	Value	Unit	Source
gf	-608.95	kJ/mol	Joback Method
hf	-1007.92	kJ/mol	Joback Method
hfus	31.03	kJ/mol	Joback Method
hvap	61.25	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.647		Crippen Method
mcvol	210.680	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	1591.00		NIST Webbook
rinpol	1591.00		NIST Webbook
tb	647.81	K	Joback Method
tc	823.38	K	Joback Method
tf	351.18	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.24	J/mol×K	647.81	Joback Method
cpg	592.31	J/mol×K	677.07	Joback Method
cpg	606.68	J/mol×K	706.33	Joback Method
cpg	620.37	J/mol×K	735.59	Joback Method
cpg	633.36	J/mol×K	764.85	Joback Method
cpg	645.67	J/mol×K	794.11	Joback Method
cpg	657.30	J/mol×K	823.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393706&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