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

Inchi: InChI=1S/C12H21FO4/c1-9(2)10(3)17-12(15)6-4-5-11(14)16-8-7-13/h9-10H,4-8H2,1-3H3

InchiKey: HXPOGEMLMJBKNG-UHFFFAOYSA-N

Formula: C12H21FO4

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

Mol. weight [g/mol]: 248.29

Physical Properties

Property code	Value	Unit	Source
gf	-617.37	kJ/mol	Joback Method
hf	-987.28	kJ/mol	Joback Method
hfus	28.44	kJ/mol	Joback Method
hvap	59.03	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.257		Crippen Method
mcvol	196.590	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	1513.00		NIST Webbook
tb	624.93	K	Joback Method
tc	801.33	K	Joback Method
tf	339.91	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.85	J/mol×K	624.93	Joback Method
cpg	539.36	J/mol×K	654.33	Joback Method
cpg	553.22	J/mol×K	683.73	Joback Method
cpg	566.43	J/mol×K	713.13	Joback Method
cpg	579.00	J/mol×K	742.53	Joback Method
cpg	590.92	J/mol×K	771.93	Joback Method
cpg	602.20	J/mol×K	801.33	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=U393705&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