Glutaric acid, 3-methylbut-2-en-1-yl 2-fluoroethyl ester

Inchi: InChI=1S/C12H19FO4/c1-10(2)6-8-16-11(14)4-3-5-12(15)17-9-7-13/h6H,3-5,7-9H2,1-2H

InchiKey: MFKRYSSUOZZWSN-UHFFFAOYSA-N

Formula: C12H19FO4

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

Mol. weight [g/mol]: 246.28

Physical Properties

Property code	Value	Unit	Source
gf	-540.82	kJ/mol	Joback Method
hf	-869.29	kJ/mol	Joback Method
hfus	34.38	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.179		Crippen Method
mcvol	192.290	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
tb	629.85	K	Joback Method
tc	809.01	K	Joback Method
tf	350.87	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.83	J/mol×K	629.85	Joback Method
cpg	516.49	J/mol×K	659.71	Joback Method
cpg	529.52	J/mol×K	689.57	Joback Method
cpg	541.93	J/mol×K	719.43	Joback Method
cpg	553.71	J/mol×K	749.29	Joback Method
cpg	564.89	J/mol×K	779.15	Joback Method
cpg	575.48	J/mol×K	809.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393707&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

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