Glutaric acid, cyclohexylmethyl 2-fluoroethyl ester

Inchi: InChI=1S/C14H23FO4/c15-9-10-18-13(16)7-4-8-14(17)19-11-12-5-2-1-3-6-12/h12H,1-11

InchiKey: CHIFWLVFZDHEHC-UHFFFAOYSA-N

Formula: C14H23FO4

SMILES: O=C(CCCC(=O)OCC1CCCCC1)OCCF

Mol. weight [g/mol]: 274.33

Physical Properties

Property code	Value	Unit	Source
gf	-571.20	kJ/mol	Joback Method
hf	-963.68	kJ/mol	Joback Method
hfus	32.50	kJ/mol	Joback Method
hvap	64.68	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.793		Crippen Method
mcvol	213.910	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	1876.00		NIST Webbook
rinpol	1876.00		NIST Webbook
tb	691.12	K	Joback Method
tc	883.63	K	Joback Method
tf	399.83	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.80	J/mol×K	691.12	Joback Method
cpg	640.98	J/mol×K	723.21	Joback Method
cpg	657.16	J/mol×K	755.29	Joback Method
cpg	672.36	J/mol×K	787.38	Joback Method
cpg	686.58	J/mol×K	819.46	Joback Method
cpg	699.83	J/mol×K	851.55	Joback Method
cpg	712.12	J/mol×K	883.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393713&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