Glutaric acid, cyclopentyl 2-fluorophenyl ester

Inchi: InChI=1S/C16H19FO4/c17-13-8-3-4-9-14(13)21-16(19)11-5-10-15(18)20-12-6-1-2-7-12/h
InchiKey: XYOMBWIEOLOTBP-UHFFFAOYSA-N
Formula: C16H19FO4
SMILES: O=C(CCCC(=O)OC1CCCC1)Oc1ccccc1F
Mol. weight [g/mol]: 294.32

Physical Properties

Property code	Value	Unit	Source
gf	-439.48	kJ/mol	Joback Method
hf	-773.74	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	71.90	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.387		Crippen Method
mcvol	218.330	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	764.27	K	Joback Method
tc	979.67	K	Joback Method
tf	464.83	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.50	J/mol×K	764.27	Joback Method
cpg	662.21	J/mol×K	800.17	Joback Method
cpg	676.72	J/mol×K	836.07	Joback Method
cpg	690.07	J/mol×K	871.97	Joback Method
cpg	702.29	J/mol×K	907.87	Joback Method
cpg	713.39	J/mol×K	943.77	Joback Method
cpg	723.42	J/mol×K	979.67	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=U405393&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