Glutaric acid, 1-cyclopentylethyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C15H22F4O4/c1-10(11-5-2-3-6-11)23-13(21)8-4-7-12(20)22-9-15(18,19)14(16

InchiKey: PJARUQGJJVBANL-UHFFFAOYSA-N

Formula: C15H22F4O4

SMILES: CC(OC(=O)CCCC(=O)OCC(F)(F)C(F)F)C1CCCC1

Mol. weight [g/mol]: 342.33

Physical Properties

Property code	Value	Unit	Source
gf	-1137.15	kJ/mol	Joback Method
hf	-1585.80	kJ/mol	Joback Method
hfus	31.97	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.722		Crippen Method
mcvol	233.310	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	1713.00		NIST Webbook
rinpol	1713.00		NIST Webbook
tb	703.43	K	Joback Method
tc	884.63	K	Joback Method
tf	388.81	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.12	J/mol×K	703.43	Joback Method
cpg	719.15	J/mol×K	733.63	Joback Method
cpg	734.23	J/mol×K	763.83	Joback Method
cpg	748.38	J/mol×K	794.03	Joback Method
cpg	761.63	J/mol×K	824.23	Joback Method
cpg	774.01	J/mol×K	854.43	Joback Method
cpg	785.54	J/mol×K	884.63	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=U405455&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