Glutaric acid, 1-cyclopentylethyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C15H23F3O4/c1-10(12-6-3-4-7-12)21-13(19)8-5-9-14(20)22-11(2)15(16,17)18

InchiKey: YAJZLSJZUNNAPV-UHFFFAOYSA-N

Formula: C15H23F3O4

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

Mol. weight [g/mol]: 324.34

Physical Properties

Property code	Value	Unit	Source
gf	-942.34	kJ/mol	Joback Method
hf	-1389.69	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	63.03	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.773		Crippen Method
mcvol	231.540	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	1632.00		NIST Webbook
tb	704.16	K	Joback Method
tc	891.07	K	Joback Method
tf	388.22	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.31	J/mol×K	704.16	Joback Method
cpg	711.91	J/mol×K	735.31	Joback Method
cpg	727.49	J/mol×K	766.46	Joback Method
cpg	742.10	J/mol×K	797.62	Joback Method
cpg	755.77	J/mol×K	828.77	Joback Method
cpg	768.51	J/mol×K	859.92	Joback Method
cpg	780.37	J/mol×K	891.07	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=U405454&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