Glutaric acid, cyclohexylmethyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C15H22F4O4/c16-14(17)15(18,19)10-23-13(21)8-4-7-12(20)22-9-11-5-2-1-3-6

InchiKey: DYAVSACZYUFVCS-UHFFFAOYSA-N

Formula: C15H22F4O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)F)OCC1CCCCC1

Mol. weight [g/mol]: 342.33

Physical Properties

Property code	Value	Unit	Source
gf	-1146.81	kJ/mol	Joback Method
hf	-1586.68	kJ/mol	Joback Method
hfus	33.40	kJ/mol	Joback Method
hvap	62.77	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.724		Crippen Method
mcvol	233.310	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook
tb	708.14	K	Joback Method
tc	891.08	K	Joback Method
tf	400.29	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.69	J/mol×K	708.14	Joback Method
cpg	722.03	J/mol×K	738.63	Joback Method
cpg	737.37	J/mol×K	769.12	Joback Method
cpg	751.73	J/mol×K	799.61	Joback Method
cpg	765.14	J/mol×K	830.10	Joback Method
cpg	777.63	J/mol×K	860.59	Joback Method
cpg	789.21	J/mol×K	891.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393662&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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