Glutaric acid, isobutyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C14H18F8O4/c1-8(2)6-25-9(23)4-3-5-10(24)26-7-12(17,18)14(21,22)13(19,20)

InchiKey: DJCFTHCYISVLAI-UHFFFAOYSA-N

Formula: C14H18F8O4

SMILES: CC(C)COC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 402.28

Physical Properties

Property code	Value	Unit	Source
gf	-1955.68	kJ/mol	Joback Method
hf	-2427.58	kJ/mol	Joback Method
hfus	32.94	kJ/mol	Joback Method
hvap	53.87	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.070		Crippen Method
mcvol	237.160	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	1577.00		NIST Webbook
tb	655.89	K	Joback Method
tc	814.74	K	Joback Method
tf	373.84	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.55	J/mol×K	655.89	Joback Method
cpg	707.97	J/mol×K	682.36	Joback Method
cpg	720.63	J/mol×K	708.84	Joback Method
cpg	732.55	J/mol×K	735.31	Joback Method
cpg	743.78	J/mol×K	761.79	Joback Method
cpg	754.34	J/mol×K	788.26	Joback Method
cpg	764.27	J/mol×K	814.74	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=U359677&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