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

Inchi: InChI=1S/C18H24F8O4/c1-10-6-7-12(8-11(10)2)30-14(28)5-3-4-13(27)29-9-16(21,22)18

InchiKey: HUIHTCHTSPSIOY-UHFFFAOYSA-N

Formula: C18H24F8O4

SMILES: CC1CCC(OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)CC1C

Mol. weight [g/mol]: 456.37

Physical Properties

Property code	Value	Unit	Source
gf	-1910.53	kJ/mol	Joback Method
hf	-2491.22	kJ/mol	Joback Method
hfus	40.80	kJ/mol	Joback Method
hvap	62.97	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.239		Crippen Method
mcvol	282.660	ml/mol	McGowan Method
pc	1103.74	kPa	Joback Method
rinpol	1922.00		NIST Webbook
rinpol	1922.00		NIST Webbook
tb	758.06	K	Joback Method
tc	934.90	K	Joback Method
tf	432.82	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.01	J/mol×K	758.06	Joback Method
cpg	933.56	J/mol×K	787.53	Joback Method
cpg	948.99	J/mol×K	817.01	Joback Method
cpg	963.38	J/mol×K	846.48	Joback Method
cpg	976.74	J/mol×K	875.95	Joback Method
cpg	989.14	J/mol×K	905.43	Joback Method
cpg	1000.62	J/mol×K	934.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405429&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