Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C18H18F8O6/c1-29-10-5-3-6-11(30-2)14(10)32-13(28)8-4-7-12(27)31-9-16(21

InchiKey: MHWXXYILMWJQJY-UHFFFAOYSA-N

Formula: C18H18F8O6

SMILES: COc1cccc(OC)c1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 482.32

Physical Properties

Property code	Value	Unit	Source
gf	-2036.41	kJ/mol	Joback Method
hf	-2555.71	kJ/mol	Joback Method
hfus	42.46	kJ/mol	Joback Method
hvap	71.58	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.494		Crippen Method
mcvol	281.500	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
rinpol	2181.00		NIST Webbook
tb	829.33	K	Joback Method
tc	1017.60	K	Joback Method
tf	529.84	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.57	J/mol×K	829.33	Joback Method
cpg	893.83	J/mol×K	860.71	Joback Method
cpg	905.12	J/mol×K	892.09	Joback Method
cpg	915.45	J/mol×K	923.47	Joback Method
cpg	924.87	J/mol×K	954.85	Joback Method
cpg	933.42	J/mol×K	986.23	Joback Method
cpg	941.13	J/mol×K	1017.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391997&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