Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C18H18F8O5/c1-10-6-7-11(29-2)12(8-10)31-14(28)5-3-4-13(27)30-9-16(21,22)17(23,24)18(25,26)15(19)20/h6-8,15H,3-5,9H2,1-2H3

InchiKey: PIXGJDUBTOBLRJ-UHFFFAOYSA-N

Formula: C18H18F8O5

SMILES: COc1ccc(C)cc1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 466.32

Physical Properties

Property code	Value	Unit	Source
gf	-1931.41	kJ/mol	Joback Method
hf	-2423.49	kJ/mol	Joback Method
hfus	41.28	kJ/mol	Joback Method
hvap	69.17	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	4.794		Crippen Method
mcvol	275.630	ml/mol	McGowan Method
pc	1218.29	kPa	Joback Method
rinpol	2088.00		NIST Webbook
rinpol	2088.00		NIST Webbook
tb	806.91	K	Joback Method
tc	992.18	K	Joback Method
tf	507.61	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.19	J/mol×K	806.91	Joback Method
cpg	866.74	J/mol×K	837.79	Joback Method
cpg	878.35	J/mol×K	868.67	Joback Method
cpg	889.08	J/mol×K	899.55	Joback Method
cpg	898.97	J/mol×K	930.43	Joback Method
cpg	908.06	J/mol×K	961.31	Joback Method
cpg	916.41	J/mol×K	992.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393920&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