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

Inchi: InChI=1S/C18H18F8O5/c1-29-12-7-5-11(6-8-12)9-30-13(27)3-2-4-14(28)31-10-16(21,22

InchiKey: WVHTUUQVMCBDOM-UHFFFAOYSA-N

Formula: C18H18F8O5

SMILES: COc1ccc(COC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)cc1

Mol. weight [g/mol]: 466.32

Physical Properties

Property code	Value	Unit	Source
gf	-1921.78	kJ/mol	Joback Method
hf	-2412.02	kJ/mol	Joback Method
hfus	41.66	kJ/mol	Joback Method
hvap	68.51	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.623		Crippen Method
mcvol	275.630	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	801.93	K	Joback Method
tc	986.25	K	Joback Method
tf	495.09	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.21	J/mol×K	801.93	Joback Method
cpg	867.84	J/mol×K	832.65	Joback Method
cpg	879.53	J/mol×K	863.37	Joback Method
cpg	890.33	J/mol×K	894.09	Joback Method
cpg	900.30	J/mol×K	924.81	Joback Method
cpg	909.47	J/mol×K	955.53	Joback Method
cpg	917.90	J/mol×K	986.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391738&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