Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C17H15F9O5/c1-29-11-7-9(18)5-6-10(11)31-13(28)4-2-3-12(27)30-8-15(21,22

InchiKey: CYVWPWBOQAEMEA-UHFFFAOYSA-N

Formula: C17H15F9O5

SMILES: COc1cc(F)ccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 470.28

Physical Properties

Property code	Value	Unit	Source
gf	-2134.64	kJ/mol	Joback Method
hf	-2598.96	kJ/mol	Joback Method
hfus	41.77	kJ/mol	Joback Method
hvap	66.13	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.624		Crippen Method
mcvol	263.310	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	1975.00		NIST Webbook
rinpol	1975.00		NIST Webbook
tb	783.30	K	Joback Method
tc	963.59	K	Joback Method
tf	496.93	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.04	J/mol×K	783.30	Joback Method
cpg	817.95	J/mol×K	813.35	Joback Method
cpg	828.98	J/mol×K	843.40	Joback Method
cpg	839.17	J/mol×K	873.44	Joback Method
cpg	848.57	J/mol×K	903.49	Joback Method
cpg	857.22	J/mol×K	933.54	Joback Method
cpg	865.16	J/mol×K	963.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393438&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

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