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

Inchi: InChI=1S/C17H16F8O5/c1-28-10-5-2-3-6-11(10)30-13(27)8-4-7-12(26)29-9-15(20,21)17

InchiKey: LWXWDYXEIBGFPU-UHFFFAOYSA-N

Formula: C17H16F8O5

SMILES: COc1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 452.29

Physical Properties

Property code	Value	Unit	Source
gf	-1930.20	kJ/mol	Joback Method
hf	-2391.38	kJ/mol	Joback Method
hfus	39.07	kJ/mol	Joback Method
hvap	66.28	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.485		Crippen Method
mcvol	261.540	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2020.00		NIST Webbook
rinpol	2020.00		NIST Webbook
tb	779.05	K	Joback Method
tc	961.25	K	Joback Method
tf	483.82	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.45	J/mol×K	779.05	Joback Method
cpg	811.72	J/mol×K	809.42	Joback Method
cpg	823.08	J/mol×K	839.78	Joback Method
cpg	833.58	J/mol×K	870.15	Joback Method
cpg	843.27	J/mol×K	900.52	Joback Method
cpg	852.19	J/mol×K	930.88	Joback Method
cpg	860.38	J/mol×K	961.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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