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

Inchi: InChI=1S/C18H16F8O5/c1-10(27)11-5-7-12(8-6-11)31-14(29)4-2-3-13(28)30-9-16(21,22
InchiKey: OSPWJLINCCDNPD-UHFFFAOYSA-N
Formula: C18H16F8O5
SMILES: CC(=O)c1ccc(OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)cc1
Mol. weight [g/mol]: 464.30

Physical Properties

Property code	Value	Unit	Source
gf	-1945.70	kJ/mol	Joback Method
hf	-2392.38	kJ/mol	Joback Method
hfus	42.08	kJ/mol	Joback Method
hvap	72.85	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.679		Crippen Method
mcvol	271.330	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	2257.00		NIST Webbook
rinpol	2257.00		NIST Webbook
tb	833.38	K	Joback Method
tc	1024.58	K	Joback Method
tf	522.79	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.70	J/mol×K	833.38	Joback Method
cpg	853.07	J/mol×K	865.25	Joback Method
cpg	863.54	J/mol×K	897.11	Joback Method
cpg	873.18	J/mol×K	928.98	Joback Method
cpg	882.04	J/mol×K	960.85	Joback Method
cpg	890.19	J/mol×K	992.72	Joback Method
cpg	897.70	J/mol×K	1024.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392029&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