Glutaric acid, 2-fluorophenyl pentafluorobenzyl ester

Inchi: InChI=1S/C18H12F6O4/c19-10-4-1-2-5-11(10)28-13(26)7-3-6-12(25)27-8-9-14(20)16(22

InchiKey: MZOOUYPGBMEAOX-UHFFFAOYSA-N

Formula: C18H12F6O4

SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 406.28

Physical Properties

Property code	Value	Unit	Source
gf	-1368.98	kJ/mol	Joback Method
hf	-1676.87	kJ/mol	Joback Method
hfus	52.18	kJ/mol	Joback Method
hvap	77.60	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	4.340		Crippen Method
mcvol	242.460	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	2208.00		NIST Webbook
rinpol	2208.00		NIST Webbook
tb	842.68	K	Joback Method
tc	1040.56	K	Joback Method
tf	568.44	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.61	J/mol×K	842.68	Joback Method
cpg	717.48	J/mol×K	875.66	Joback Method
cpg	727.42	J/mol×K	908.64	Joback Method
cpg	736.44	J/mol×K	941.62	Joback Method
cpg	744.53	J/mol×K	974.60	Joback Method
cpg	751.70	J/mol×K	1007.58	Joback Method
cpg	757.95	J/mol×K	1040.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391934&Units=SI

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