Glutaric acid, ethyl pentafluorobenzyl ester

Inchi: InChI=1S/C14H13F5O4/c1-2-22-8(20)4-3-5-9(21)23-6-7-10(15)12(17)14(19)13(18)11(7)1
InchiKey: ZGTOBDXEPVNSDX-UHFFFAOYSA-N
Formula: C14H13F5O4
SMILES: CCOC(=O)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 340.24

Physical Properties

Property code	Value	Unit	Source
gf	-1310.63	kJ/mol	Joback Method
hf	-1623.26	kJ/mol	Joback Method
hfus	45.09	kJ/mol	Joback Method
hvap	66.57	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.159		Crippen Method
mcvol	208.090	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	1774.00		NIST Webbook
rinpol	1774.00		NIST Webbook
tb	720.23	K	Joback Method
tc	898.40	K	Joback Method
tf	483.83	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.44	J/mol×K	720.23	Joback Method
cpg	586.93	J/mol×K	749.93	Joback Method
cpg	597.79	J/mol×K	779.62	Joback Method
cpg	608.03	J/mol×K	809.32	Joback Method
cpg	617.63	J/mol×K	839.01	Joback Method
cpg	626.58	J/mol×K	868.71	Joback Method
cpg	634.88	J/mol×K	898.40	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=U358865&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