Glutaric acid, ethyl pentafluorophenyl ester

Inchi: InChI=1S/C13H11F5O4/c1-2-21-6(19)4-3-5-7(20)22-13-11(17)9(15)8(14)10(16)12(13)18
InchiKey: ZDRSJTSCTLYWMD-UHFFFAOYSA-N
Formula: C13H11F5O4
SMILES: CCOC(=O)CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 326.22

Physical Properties

Property code	Value	Unit	Source
gf	-1319.05	kJ/mol	Joback Method
hf	-1602.62	kJ/mol	Joback Method
hfus	42.50	kJ/mol	Joback Method
hvap	64.34	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.021		Crippen Method
mcvol	194.000	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	1602.00		NIST Webbook
tb	697.35	K	Joback Method
tc	875.33	K	Joback Method
tf	472.56	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.24	J/mol×K	697.35	Joback Method
cpg	534.14	J/mol×K	727.01	Joback Method
cpg	544.47	J/mol×K	756.68	Joback Method
cpg	554.22	J/mol×K	786.34	Joback Method
cpg	563.39	J/mol×K	816.00	Joback Method
cpg	571.97	J/mol×K	845.67	Joback Method
cpg	579.94	J/mol×K	875.33	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=U359064&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