Diglycolic acid, ethyl pentafluorobenzyl ester

Inchi: InChI=1S/C13H11F5O5/c1-2-22-7(19)4-21-5-8(20)23-3-6-9(14)11(16)13(18)12(17)10(6)1
InchiKey: FQMZPWKDJJSYID-UHFFFAOYSA-N
Formula: C13H11F5O5
SMILES: CCOC(=O)COCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 342.22

Physical Properties

Property code	Value	Unit	Source
gf	-1424.05	kJ/mol	Joback Method
hf	-1734.84	kJ/mol	Joback Method
hfus	43.68	kJ/mol	Joback Method
hvap	66.75	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.005		Crippen Method
mcvol	199.870	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	719.77	K	Joback Method
tc	898.41	K	Joback Method
tf	494.79	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.61	J/mol×K	719.77	Joback Method
cpg	559.45	J/mol×K	749.54	Joback Method
cpg	569.69	J/mol×K	779.32	Joback Method
cpg	579.31	J/mol×K	809.09	Joback Method
cpg	588.30	J/mol×K	838.87	Joback Method
cpg	596.63	J/mol×K	868.64	Joback Method
cpg	604.30	J/mol×K	898.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382069&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