Diglycolic acid, pentafluorobenzyl propyl ester

Inchi: InChI=1S/C14H13F5O5/c1-2-3-23-8(20)5-22-6-9(21)24-4-7-10(15)12(17)14(19)13(18)11
InchiKey: NCTBBOHGBONYDK-UHFFFAOYSA-N
Formula: C14H13F5O5
SMILES: CCCOC(=O)COCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 356.24

Physical Properties

Property code	Value	Unit	Source
gf	-1415.63	kJ/mol	Joback Method
hf	-1755.48	kJ/mol	Joback Method
hfus	46.27	kJ/mol	Joback Method
hvap	68.98	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.395		Crippen Method
mcvol	213.960	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	742.65	K	Joback Method
tc	921.94	K	Joback Method
tf	506.06	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.51	J/mol×K	742.65	Joback Method
cpg	612.91	J/mol×K	772.53	Joback Method
cpg	623.65	J/mol×K	802.41	Joback Method
cpg	633.71	J/mol×K	832.30	Joback Method
cpg	643.07	J/mol×K	862.18	Joback Method
cpg	651.71	J/mol×K	892.06	Joback Method
cpg	659.63	J/mol×K	921.94	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=U382070&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