Diglycolic acid, isobutyl pentafluorobenzyl ester

Inchi: InChI=1S/C15H15F5O5/c1-7(2)3-24-9(21)5-23-6-10(22)25-4-8-11(16)13(18)15(20)14(19

InchiKey: UDCCKKOZPLOWHA-UHFFFAOYSA-N

Formula: C15H15F5O5

SMILES: CC(C)COC(=O)COCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 370.27

Physical Properties

Property code	Value	Unit	Source
gf	-1409.65	kJ/mol	Joback Method
hf	-1781.40	kJ/mol	Joback Method
hfus	45.34	kJ/mol	Joback Method
hvap	70.82	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	2.641		Crippen Method
mcvol	228.050	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2272.00		NIST Webbook
rinpol	2272.00		NIST Webbook
tb	765.09	K	Joback Method
tc	947.06	K	Joback Method
tf	502.33	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.14	J/mol×K	765.09	Joback Method
cpg	668.17	J/mol×K	795.42	Joback Method
cpg	679.45	J/mol×K	825.75	Joback Method
cpg	689.96	J/mol×K	856.08	Joback Method
cpg	699.68	J/mol×K	886.40	Joback Method
cpg	708.61	J/mol×K	916.73	Joback Method
cpg	716.72	J/mol×K	947.06	Joback Method

Sources

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=U382071&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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