Diglycolic acid, di(pentafluorobenzyl) ester

Inchi: InChI=1S/C18H8F10O5/c19-9-5(10(20)14(24)17(27)13(9)23)1-32-7(29)3-31-4-8(30)33-2
InchiKey: OLMOTAQHFRKKQH-UHFFFAOYSA-N
Formula: C18H8F10O5
SMILES: O=C(COCC(=O)OCc1c(F)c(F)c(F)c(F)c1F)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 494.24

Physical Properties

Property code	Value	Unit	Source
gf	-2291.74	kJ/mol	Joback Method
hf	-2639.41	kJ/mol	Joback Method
hfus	64.13	kJ/mol	Joback Method
hvap	79.39	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	3.881		Crippen Method
mcvol	255.410	ml/mol	McGowan Method
pc	1267.35	kPa	Joback Method
rinpol	2647.00		NIST Webbook
rinpol	2647.00		NIST Webbook
tb	882.10	K	Joback Method
tc	1079.94	K	Joback Method
tf	643.11	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.88	J/mol×K	882.10	Joback Method
cpg	765.31	J/mol×K	915.07	Joback Method
cpg	773.69	J/mol×K	948.05	Joback Method
cpg	781.02	J/mol×K	981.02	Joback Method
cpg	787.27	J/mol×K	1014.00	Joback Method
cpg	792.41	J/mol×K	1046.97	Joback Method
cpg	796.41	J/mol×K	1079.94	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=U382086&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