

Diglycolic acid, isohexyl pentafluorobenzyl ester

Inchi:	InChI=1S/C17H19F5O5/c1-9(2)4-3-5-26-11(23)7-25-8-12(24)27-6-10-13(18)15(20)17(22)
InchiKey:	YHYOSVSPNPDGNN-UHFFFAOYSA-N
Formula:	C17H19F5O5
SMILES:	CC(C)CCCOC(=O)COCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	398.32

Physical Properties

Property code	Value	Unit	Source
gf	-1392.81	kJ/mol	Joback Method
hf	-1822.68	kJ/mol	Joback Method
hfus	50.52	kJ/mol	Joback Method
hvap	75.27	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.421		Crippen Method
mcvol	256.230	ml/mol	McGowan Method
pc	1335.88	kPa	Joback Method
rinpola	2521.00		NIST Webbook
rinpola	2521.00		NIST Webbook
tb	810.85	K	Joback Method
tc	996.64	K	Joback Method
tf	524.87	K	Joback Method
vc	1.030	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.40	J/molxK	810.85	Joback Method
cpg	780.34	J/molxK	841.82	Joback Method
cpg	792.37	J/molxK	872.78	Joback Method
cpg	803.48	J/molxK	903.75	Joback Method
cpg	813.67	J/molxK	934.71	Joback Method
cpg	822.93	J/molxK	965.68	Joback Method
cpg	831.23	J/molxK	996.64	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U382074&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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