Diglycolic acid, hexyl pentafluorobenzyl ester

Inchi: InChI=1S/C17H19F5O5/c1-2-3-4-5-6-26-11(23)8-25-9-12(24)27-7-10-13(18)15(20)17(22
InchiKey: MQVOXGNYFNWQTH-UHFFFAOYSA-N
Formula: C17H19F5O5
SMILES: CCCCCCOC(=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	-1390.37	kJ/mol	Joback Method
hf	-1817.40	kJ/mol	Joback Method
hfus	54.04	kJ/mol	Joback Method
hvap	75.66	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.565		Crippen Method
mcvol	256.230	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	2566.00		NIST Webbook
rinpol	2566.00		NIST Webbook
tb	811.29	K	Joback Method
tc	996.24	K	Joback Method
tf	539.87	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.85	J/mol×K	811.29	Joback Method
cpg	779.72	J/mol×K	842.11	Joback Method
cpg	791.71	J/mol×K	872.94	Joback Method
cpg	802.80	J/mol×K	903.76	Joback Method
cpg	812.98	J/mol×K	934.59	Joback Method
cpg	822.25	J/mol×K	965.41	Joback Method
cpg	830.58	J/mol×K	996.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382075&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

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