

Diglycolic acid, decyl pentafluorobenzyl ester

Inchi:	InChI=1S/C21H27F5O5/c1-2-3-4-5-6-7-8-9-10-30-15(27)12-29-13-16(28)31-11-14-17(22)
InchiKey:	ZSJMGSIWZGNAHZ-UHFFFAOYSA-N
Formula:	C21H27F5O5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	454.43

Physical Properties

Property code	Value	Unit	Source
gf	-1356.69	kJ/mol	Joback Method
hf	-1899.96	kJ/mol	Joback Method
hfus	64.40	kJ/mol	Joback Method
hvap	84.56	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	5.126		Crippen Method
mvol	312.590	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	3053.00		NIST Webbook
rinpol	3053.00		NIST Webbook
tb	902.81	K	Joback Method
tc	1106.22	K	Joback Method
tf	584.95	K	Joback Method
vc	1.260	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.57	J/mol×K	902.81	Joback Method
cpg	1014.16	J/mol×K	936.71	Joback Method
cpg	1027.44	J/mol×K	970.61	Joback Method
cpg	1039.42	J/mol×K	1004.51	Joback Method
cpg	1050.08	J/mol×K	1038.41	Joback Method
cpg	1059.43	J/mol×K	1072.31	Joback Method
cpg	1067.46	J/mol×K	1106.22	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=U382079&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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