

Diglycolic acid, dodecyl pentafluorobenzyl ester

Inchi:	InChI=1S/C23H31F5O5/c1-2-3-4-5-6-7-8-9-10-11-12-32-17(29)14-31-15-18(30)33-13-16
InchiKey:	QSLMEEUERBWNFJ-UHFFFAOYSA-N
Formula:	C23H31F5O5
SMILES:	CCCCCCCCCCCCOC(=O)COCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	482.48

Physical Properties

Property code	Value	Unit	Source
gf	-1339.85	kJ/mol	Joback Method
hf	-1941.24	kJ/mol	Joback Method
hfus	69.58	kJ/mol	Joback Method
hvap	89.02	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	5.906		Crippen Method
mvol	340.770	ml/mol	McGowan Method
pc	907.24	kPa	Joback Method
rinpol	3286.00		NIST Webbook
rinpol	3286.00		NIST Webbook
tb	948.57	K	Joback Method
tc	1167.15	K	Joback Method
tf	607.49	K	Joback Method
vc	1.371	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.78	J/molxK	948.57	Joback Method
cpg	1135.20	J/molxK	985.00	Joback Method
cpg	1149.01	J/molxK	1021.43	Joback Method
cpg	1161.20	J/molxK	1057.86	Joback Method
cpg	1171.79	J/molxK	1094.29	Joback Method
cpg	1180.77	J/molxK	1130.72	Joback Method
cpg	1188.14	J/molxK	1167.15	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=U382081&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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