Diglycolic acid, pentafluorobenzyl undecyl ester

Inchi: InChI=1S/C22H29F5O5/c1-2-3-4-5-6-7-8-9-10-11-31-16(28)13-30-14-17(29)32-12-15-18
InchiKey: ZMJMNBUTFSJQNZ-UHFFFAOYSA-N
Formula: C22H29F5O5
SMILES: CCCCCCCCCCCOC(=O)COCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 468.45

Physical Properties

Property code	Value	Unit	Source
gf	-1348.27	kJ/mol	Joback Method
hf	-1920.60	kJ/mol	Joback Method
hfus	66.99	kJ/mol	Joback Method
hvap	86.79	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	5.516		Crippen Method
mcvol	326.680	ml/mol	McGowan Method
pc	962.08	kPa	Joback Method
rinpol	3172.00		NIST Webbook
rinpol	3172.00		NIST Webbook
tb	925.69	K	Joback Method
tc	1136.12	K	Joback Method
tf	596.22	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.42	J/mol×K	925.69	Joback Method
cpg	1074.42	J/mol×K	960.76	Joback Method
cpg	1087.98	J/mol×K	995.83	Joback Method
cpg	1100.09	J/mol×K	1030.91	Joback Method
cpg	1110.74	J/mol×K	1065.98	Joback Method
cpg	1119.95	J/mol×K	1101.05	Joback Method
cpg	1127.70	J/mol×K	1136.12	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382080&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
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