DOPA, HFIP-PFP

Inchi: InChI=1S/C21H8F21NO7/c22-14(23,19(34,35)36)11(45)43-6(9(44)50-10(17(28,29)30)18
InchiKey: IBBQYKLYEGERBB-UHFFFAOYSA-N
Formula: C21H8F21NO7
SMILES: O=C(OC(C(F)(F)F)C(F)(F)F)C(Cc1ccc(OC(=O)C(F)(F)C(F)(F)F)c(OC(=O)C(F)(F)C(F)(F)
Mol. weight [g/mol]: 785.26

Physical Properties

Property code	Value	Unit	Source
gf	-4595.37	kJ/mol	Joback Method
hf	-5255.56	kJ/mol	Joback Method
hfus	56.79	kJ/mol	Joback Method
hvap	78.29	kJ/mol	Joback Method
log10ws	-8.97		Crippen Method
logp	6.154		Crippen Method
mcvol	354.030	ml/mol	McGowan Method
pc	818.20	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1386.00		NIST Webbook
tb	1007.38	K	Joback Method
tc	1270.84	K	Joback Method
tf	698.71	K	Joback Method
vc	1.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1189.56	J/mol×K	1007.38	Joback Method
cpg	1199.00	J/mol×K	1051.29	Joback Method
cpg	1207.97	J/mol×K	1095.20	Joback Method
cpg	1216.82	J/mol×K	1139.11	Joback Method
cpg	1225.93	J/mol×K	1183.02	Joback Method
cpg	1235.65	J/mol×K	1226.93	Joback Method
cpg	1246.36	J/mol×K	1270.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57149&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