Dihydroxyphenylalanine, TFE-PFP

Other names: DOPA, TFE-PFP
Inchi: InChI=1S/C20H9F18NO7/c21-14(22,23)5-44-10(40)7(39-11(41)15(24,25)18(30,31)32)3-
InchiKey: GFFAEDKYDRYONH-UHFFFAOYSA-N
Formula: C20H9F18NO7
SMILES: O=C(OCC(F)(F)F)C(Cc1ccc(OC(=O)C(F)(F)C(F)(F)F)c(OC(=O)C(F)(F)C(F)(F)F)c1)NC(=
Mol. weight [g/mol]: 717.26

Physical Properties

Property code	Value	Unit	Source
gf	-4019.76	kJ/mol	Joback Method
hf	-4632.56	kJ/mol	Joback Method
hfus	55.90	kJ/mol	Joback Method
hvap	80.20	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	5.223		Crippen Method
mcvol	334.630	ml/mol	McGowan Method
pc	922.74	kPa	Joback Method
rinpol	1548.00		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1548.00		NIST Webbook
tb	990.36	K	Joback Method
tc	1233.43	K	Joback Method
tf	698.25	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1110.93	J/mol×K	990.36	Joback Method
cpg	1119.70	J/mol×K	1030.87	Joback Method
cpg	1127.81	J/mol×K	1071.38	Joback Method
cpg	1135.52	J/mol×K	1111.90	Joback Method
cpg	1143.07	J/mol×K	1152.41	Joback Method
cpg	1150.71	J/mol×K	1192.92	Joback Method

cpg	1158.69	J/mol×K	1233.43	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=R57153&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