Phe, HFIP-PFP

Other names: Phenylalanine, HFIP-PFP
Inchi: InChI=1S/C15H10F11NO3/c16-12(17,15(24,25)26)11(29)27-8(6-7-4-2-1-3-5-7)9(28)30-1
InchiKey: ZJQYABQTYMRQJI-UHFFFAOYSA-N
Formula: C15H10F11NO3
SMILES: O=C(OC(C(F)(F)F)C(F)(F)F)C(Cc1ccccc1)NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 461.23

Physical Properties

Property code	Value	Unit	Source
gf	-2222.05	kJ/mol	Joback Method
hf	-2623.08	kJ/mol	Joback Method
hfus	35.31	kJ/mol	Joback Method
hvap	58.65	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	3.948		Crippen Method
mcvol	236.910	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	1091.00		NIST Webbook
rinpol	1091.00		NIST Webbook
tb	727.78	K	Joback Method
tc	903.03	K	Joback Method
tf	446.15	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.82	J/mol×K	727.78	Joback Method
cpg	729.66	J/mol×K	756.99	Joback Method
cpg	739.62	J/mol×K	786.20	Joback Method
cpg	748.79	J/mol×K	815.41	Joback Method
cpg	757.23	J/mol×K	844.62	Joback Method
cpg	765.01	J/mol×K	873.82	Joback Method
cpg	772.21	J/mol×K	903.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57167&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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