o-Synephrine, TFA

Inchi: InChI=1S/C15H10F9NO5/c1-25(10(26)13(16,17)18)6-9(30-12(28)15(22,23)24)7-4-2-3-5-
InchiKey: OOBBYRJKEDDZTB-UHFFFAOYSA-N
Formula: C15H10F9NO5
SMILES: CN(CC(OC(=O)C(F)(F)F)c1ccccc1OC(=O)C(F)(F)F)C(=O)C(F)(F)F
Mol. weight [g/mol]: 455.23

Physical Properties

Property code	Value	Unit	Source
gf	-2054.99	kJ/mol	Joback Method
hf	-2459.04	kJ/mol	Joback Method
hfus	40.41	kJ/mol	Joback Method
hvap	67.39	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.322		Crippen Method
mcvol	240.810	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	1430.00		NIST Webbook
rinpol	1430.00		NIST Webbook
tb	776.45	K	Joback Method
tc	959.53	K	Joback Method
tf	522.04	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.19	J/mol×K	776.45	Joback Method
cpg	735.30	J/mol×K	806.96	Joback Method
cpg	744.58	J/mol×K	837.48	Joback Method
cpg	753.08	J/mol×K	867.99	Joback Method
cpg	760.86	J/mol×K	898.50	Joback Method
cpg	767.98	J/mol×K	929.01	Joback Method
cpg	774.49	J/mol×K	959.53	Joback Method

Sources

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=R529854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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