

Tyr, N-TFA

Inchi:	InChI=1S/C11H10F3NO3/c12-11(13,14)10(18)15-8(6-16)5-7-1-3-9(17)4-2-7/h1-4,6,8,17H
InchiKey:	KRQPEINSTYQVPV-UHFFFAOYSA-N
Formula:	C11H10F3NO3
SMILES:	O=CC(Cc1ccc(O)cc1)NC(=O)C(F)(F)F
Mol. weight [g/mol]:	261.20

Physical Properties

Property code	Value	Unit	Source
gf	-723.55	kJ/mol	Joback Method
hf	-958.20	kJ/mol	Joback Method
hfus	31.36	kJ/mol	Joback Method
hvap	71.14	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.181		Crippen Method
mcvol	166.390	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1597.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1601.00		NIST Webbook
rinpol	1597.00		NIST Webbook
tb	705.22	K	Joback Method
tc	915.90	K	Joback Method
tf	485.65	K	Joback Method
vc	0.605	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.25	J/molxK	705.22	Joback Method
cpg	473.23	J/molxK	740.33	Joback Method
cpg	482.48	J/molxK	775.45	Joback Method
cpg	491.09	J/molxK	810.56	Joback Method

cpg	499.17	J/mol×K	845.67	Joback Method
cpg	506.79	J/mol×K	880.78	Joback Method
cpg	514.07	J/mol×K	915.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R98060&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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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