

Tymazoline

Inchi:	InChI=1S/C14H20N2O/c1-10(2)12-5-4-11(3)8-13(12)17-9-14-15-6-7-16-14/h4-5,8,10H,6
InchiKey:	QRORCRWSRPKEHR-UHFFFAOYSA-N
Formula:	C14H20N2O
SMILES:	<chem>Cc1ccc(C(C)C)c(OCC2=NCCN2)c1</chem>
Mol. weight [g/mol]:	232.32

Physical Properties

Property code	Value	Unit	Source
gf	321.79	kJ/mol	Joback Method
hf	-20.29	kJ/mol	Joback Method
hfus	31.37	kJ/mol	Joback Method
hvap	66.87	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.499		Crippen Method
mvol	195.030	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook
tb	704.68	K	Joback Method
tc	943.74	K	Joback Method
tf	511.22	K	Joback Method
vc	0.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.17	J/mol×K	704.68	Joback Method
cpg	575.92	J/mol×K	744.52	Joback Method
cpg	593.30	J/mol×K	784.37	Joback Method
cpg	609.34	J/mol×K	824.21	Joback Method
cpg	624.03	J/mol×K	864.05	Joback Method
cpg	637.38	J/mol×K	903.90	Joback Method
cpg	649.42	J/mol×K	943.74	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=R18375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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