Tramazoline

Other names:	Tramazoline
	Imidazolidine,2-[(5,6,7,8-tetrahydronaphthal-1-yl]imino-
	2-[(5,6,7,8-Tetrahydro-1-naphthyl)amino]-2-imidazoline
	4,5-Dihydro-N-(5,6,7,8-tetrahydro-1-naphthalenyl)-1H-imidazol-2-amine
Inchi:	InChI=1S/C13H17N3/c1-2-6-11-10(4-1)5-3-7-12(11)16-13-14-8-9-15-13/h3,5,7H,1-2,4,6,8
InchiKey:	QQJLHRRUATVHED-UHFFFAOYSA-N
Formula:	C13H17N3
SMILES:	c1cc2c(c(NC3=NCCN3)c1)CCCC2
Mol. weight [g/mol]:	215.30

Physical Properties

Property code	Value	Unit	Source
hfus	31.18	kJ/mol	Joback Method
ie	7.62	eV	NIST Webbook
logp	1.937		Crippen Method
mcvol	174.190	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.94	J/mol×K	725.67	Joback Method
cpg	533.27	J/mol×K	769.75	Joback Method
cpg	550.01	J/mol×K	813.83	Joback Method
cpg	565.26	J/mol×K	857.92	Joback Method
cpg	579.10	J/mol×K	902.00	Joback Method
cpg	591.63	J/mol×K	946.08	Joback Method
cpg	602.94	J/mol×K	990.16	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1082571&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume