Cyclopropanamine, 2-phenyl-, trans-(+)-

Other names:	(+)-Tranylcypromine
	(+)-trans-2-Phenylcyclopropylamine
	(1R,2S)-rel-2-phenylcyclopropanamine
	(1S-trans)-2-Phenylcyclopropanamine
	2-Phenyl-1-aminocyclopropane, trans-
	Cyclopropylamine, 2-phenyl-, (1S-trans)-
	Cyclopropylamine, 2-phenyl-, trans-
	D-Tranylcypromine
	dl-tranylcypromine
	trans-2-phenylcyclopropylamine
Inchi:	InChI=1S/C9H11N/c10-9-6-8(9)7-4-2-1-3-5-7/h1-5,8-9H,6,10H2
InchiKey:	AELCINSCMGFISI-UHFFFAOYSA-N
Formula:	C9H11N
SMILES:	NC1CC1c1ccccc1
Mol. weight [g/mol]:	133.19
CAS:	3721-28-6

Physical Properties

Property code	Value	Unit	Source
gf	256.80	kJ/mol	Joback Method
hf	93.69	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	48.15	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.501		Crippen Method
mcvol	113.030	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
rinpol	1240.30		NIST Webbook
tb	506.60	K	Joback Method
tc	743.89	K	Joback Method
tf	314.57	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.78	J/mol×K	704.34	Joback Method
cpg	257.94	J/mol×K	506.60	Joback Method
cpg	273.48	J/mol×K	546.15	Joback Method
cpg	287.86	J/mol×K	585.70	Joback Method
cpg	301.16	J/mol×K	625.25	Joback Method
cpg	313.44	J/mol×K	664.79	Joback Method
cpg	335.27	J/mol×K	743.89	Joback Method
pvap	0.03	kPa	298.15	The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography

Sources

The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je400498a
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=C3721286&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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