Tranylcypromine

Other names:	Cyclopropanamine, 2-phenyl-, trans-(.+/-.)-
Inchi:	InChI=1S/C9H11N/c10-9-6-8(9)7-4-2-1-3-5-7/h1-5,8-9H,6,10H2/t8-,9+/m1/s1
InchiKey:	AELCINSCMGFISI-BDAKNGLRSA-N
Formula:	C9H11N
SMILES:	NC1CC1c1ccccc1
Mol. weight [g/mol]:	133.19
CAS:	155-09-9

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	1259.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1198.00		NIST Webbook
ripol	1850.00		NIST Webbook
ripol	1834.00		NIST Webbook

ripol	1904.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1852.00		NIST Webbook
ripol	1834.00		NIST Webbook
ripol	1834.00		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	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	324.78	J/mol×K	704.34	Joback Method
cpg	335.27	J/mol×K	743.89	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=C155099&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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