N-Acetyltranylcypromine

Other names: Tranylcypromine acetate
N-(2-Phenylcyclopropyl)acetamide
Tranylcypromine, acetylated
Inchi: InChI=1S/C11H13NO/c1-8(13)12-11-7-10(11)9-5-3-2-4-6-9/h2-6,10-11H,7H2,1H3,(H,12,
InchiKey: OKNYZIGDRLPEEJ-UHFFFAOYSA-N
Formula: C11H13NO
SMILES: CC(=O)NC1CC1c1ccccc1
Mol. weight [g/mol]: 175.23
CAS: 78682-61-8

Physical Properties

Property code	Value	Unit	Source
gf	167.66	kJ/mol	Joback Method
hf	-40.49	kJ/mol	Joback Method
hfus	24.19	kJ/mol	Joback Method
hvap	55.14	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	1.679		Crippen Method
mcvol	142.780	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	1636.00		NIST Webbook
rinpol	1695.00		NIST Webbook
tb	583.87	K	Joback Method
tc	810.97	K	Joback Method
tf	356.44	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.36	J/mol×K	583.87	Joback Method
cpg	374.07	J/mol×K	621.72	Joback Method
cpg	388.64	J/mol×K	659.57	Joback Method
cpg	402.16	J/mol×K	697.42	Joback Method

cpg	414.68	J/mol×K	735.27	Joback Method
cpg	426.29	J/mol×K	773.12	Joback Method
cpg	437.06	J/mol×K	810.97	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=C78682618&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume