Desmethyldeprenyl

Other names: (.+/-.)-N-Desmethylselegiline
Inchi: InChI=1S/C12H15N/c1-3-9-13-11(2)10-12-7-5-4-6-8-12/h1,4-8,11,13H,9-10H2,2H3
InchiKey: UUFAJPMQSFXDFR-UHFFFAOYSA-N
Formula: C12H15N
SMILES: C#CCNC(C)Cc1ccccc1
Mol. weight [g/mol]: 173.25
CAS: 18913-84-3

Physical Properties

Property code	Value	Unit	Source
gf	472.59	kJ/mol	Joback Method
hf	285.61	kJ/mol	Joback Method
hfus	25.43	kJ/mol	Joback Method
hvap	50.49	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	1.840		Crippen Method
mcvol	157.560	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1362.80		NIST Webbook
tb	540.49	K	Joback Method
tc	759.78	K	Joback Method
tf	336.05	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.64	J/mol×K	540.49	Joback Method
cpg	376.57	J/mol×K	577.04	Joback Method
cpg	391.46	J/mol×K	613.59	Joback Method
cpg	405.38	J/mol×K	650.14	Joback Method
cpg	418.37	J/mol×K	686.68	Joback Method
cpg	430.49	J/mol×K	723.23	Joback Method
cpg	441.79	J/mol×K	759.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18913843&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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