

Selegiline

Other names:	(R)-((-)-N,«alpha»-Dimethyl-N-2-propynylphenethylamine (-)-Deprenil Eldepryl Jumex L-Deprenyl N-Methyl-N-(1-methyl-2-phenylethyl)-2-propyn-1-amine-, L-(-)- Selegiline-, (-)- (-)-Selegiline Anipryl Benzeneethanamine, N,«alpha»-methyl-N-2-propynyl-, («alpha»R)- Benzeneethanamine, N,«alpha»-dimethyl-N-2-propyn-1-yl-, («alpha»R)- Benzeneethanamine, N,.alpha.-dimethyl-N-2-propynyl-, (R)-
Inchi:	InChI=1S/C13H17N/c1-4-10-14(3)12(2)11-13-8-6-5-7-9-13/h1,5-9,12H,10-11H2,2-3H3
InchiKey:	MEZLKOACVSPNER-UHFFFAOYSA-N
Formula:	C13H17N
SMILES:	C#CCN(C)C(C)Cc1ccccc1
Mol. weight [g/mol]:	187.28
CAS:	14611-51-9

Physical Properties

Property code	Value	Unit	Source
gf	502.40	kJ/mol	Joback Method
hf	279.03	kJ/mol	Joback Method
hfus	25.94	kJ/mol	Joback Method
hvap	48.32	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.183		Crippen Method
mcvol	171.650	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1439.70		NIST Webbook
rinpol	1439.70		NIST Webbook
tb	525.64	K	Joback Method
tc	737.90	K	Joback Method
tf	327.13	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.41	J/mol×K	525.64	Joback Method
cpg	408.98	J/mol×K	561.02	Joback Method
cpg	425.43	J/mol×K	596.39	Joback Method
cpg	440.81	J/mol×K	631.77	Joback Method
cpg	455.19	J/mol×K	667.15	Joback Method
cpg	468.62	J/mol×K	702.52	Joback Method
cpg	481.16	J/mol×K	737.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14611519&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	http://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

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