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]:	187.29

Physical Properties

Property code	Value	Unit	Source
af	0.3634		Cheméo Relay (1.0)
hf	288.31	kJ/mol	Cheméo Relay (1.0)
hfus	25.94	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Cheméo Relay (1.0)
ie	8.20	eV	Cheméo Relay (1.0)
log10ws	-1.41		Cheméo Relay (1.0)
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	532.66	K	Cheméo Relay (1.0)
tc	723.45	K	Cheméo Relay (1.0)
tf	262.81	K	Cheméo Relay (1.0)
vc	0.585	m3/kmol	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14611519&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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