7-Methyl-1,5-diazacyclotetradecane

Other names: (S)-7-methyl-1,5-diazacyclotetradecane (S-(-)-haliclorensin)
Inchi: InChI=1S/C13H28N2/c1-13-8-5-3-2-4-6-9-14-10-7-11-15-12-13/h13-15H,2-12H2,1H3
InchiKey: OFPMSWKVQNUTSL-UHFFFAOYSA-N
Formula: C13H28N2
SMILES: CC1CCCCCCCNCCCNC1
Mol. weight [g/mol]: 212.37

Physical Properties

Property code	Value	Unit	Source
gf	161.65	kJ/mol	Joback Method
hf	-230.99	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Joback Method
hvap	59.85	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.546		Crippen Method
mcvol	203.130	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	1711.00		NIST Webbook
rinpol	1711.00		NIST Webbook
tb	647.65	K	Joback Method
tc	906.72	K	Joback Method
tf	425.55	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.29	J/mol×K	647.65	Joback Method
cpg	607.04	J/mol×K	690.83	Joback Method
cpg	634.61	J/mol×K	734.01	Joback Method
cpg	659.91	J/mol×K	777.18	Joback Method
cpg	682.88	J/mol×K	820.36	Joback Method
cpg	703.44	J/mol×K	863.54	Joback Method
cpg	721.52	J/mol×K	906.72	Joback Method

Sources

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=U360451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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