Perhydroamphetamine

Inchi: InChI=1S/C9H19N/c1-8(10)7-9-5-3-2-4-6-9/h8-9H,2-7,10H2,1H3
InchiKey: GIXSTBOIKJPUKD-UHFFFAOYSA-N
Formula: C9H19N
SMILES: CC(N)CC1CCCCC1
Mol. weight [g/mol]: 141.25

Physical Properties

Property code	Value	Unit	Source
gf	113.36	kJ/mol	Joback Method
hf	-146.26	kJ/mol	Joback Method
hfus	12.57	kJ/mol	Joback Method
hvap	46.31	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.304		Crippen Method
mcvol	136.790	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1102.00		NIST Webbook
rinpol	1102.00		NIST Webbook
ripol	1366.00		NIST Webbook
tb	496.96	K	Joback Method
tc	713.33	K	Joback Method
tf	266.83	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.77	J/mol×K	496.96	Joback Method
cpg	341.88	J/mol×K	533.02	Joback Method
cpg	359.92	J/mol×K	569.08	Joback Method
cpg	376.94	J/mol×K	605.15	Joback Method
cpg	392.96	J/mol×K	641.21	Joback Method
cpg	408.02	J/mol×K	677.27	Joback Method
cpg	422.15	J/mol×K	713.33	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=R385401&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/50-299-5/Perhydroamphetamine.pdf

Generated by Cheméo on 2024-10-12 08:19:16.751391978 +0000 UTC m=+3302019.388361226.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.