

Perhydrophentermine

Inchi:	InChI=1S/C10H21N/c1-10(2,11)8-9-6-4-3-5-7-9/h9H,3-8,11H2,1-2H3
InchiKey:	KZVACGSZWDLFHD-UHFFFAOYSA-N
Formula:	C10H21N
SMILES:	CC(C)(N)CC1CCCCC1
Mol. weight [g/mol]:	155.28
CAS:	5531-31-7

Physical Properties

Property code	Value	Unit	Source
gf	127.06	kJ/mol	Joback Method
hf	-170.37	kJ/mol	Joback Method
hfus	11.27	kJ/mol	Joback Method
hvap	47.63	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.694		Crippen Method
mcvol	150.880	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1152.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1152.00		NIST Webbook
ripol	1359.00		NIST Webbook
ripol	1359.00		NIST Webbook
tb	517.05	K	Joback Method
tc	738.95	K	Joback Method
tf	295.52	K	Joback Method
vc	0.546	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.01	J/mol×K	517.05	Joback Method
cpg	393.78	J/mol×K	554.03	Joback Method
cpg	413.23	J/mol×K	591.02	Joback Method

cpg	431.41	J/mol×K	628.00	Joback Method
cpg	448.40	J/mol×K	664.99	Joback Method
cpg	464.24	J/mol×K	701.97	Joback Method
cpg	479.01	J/mol×K	738.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5531317&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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