

Decahydroquinoline, 4a-methyl

Inchi: InChI=1S/C10H19N/c1-8-6-7-11-10-5-3-2-4-9(8)10/h8-11H,2-7H2,1H3
InchiKey: WPBVRISDNZUAEU-UHFFFAOYSA-N
Formula: C10H19N
SMILES: CC1CCNC2CCCCC12
Mol. weight [g/mol]: 153.26

Physical Properties

Property code	Value	Unit	Source
gf	186.42	kJ/mol	Joback Method
hf	-111.30	kJ/mol	Joback Method
hfus	20.19	kJ/mol	Joback Method
hvap	44.82	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.175		Crippen Method
mcvol	140.020	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	1215.00		NIST Webbook
rinpol	1215.00		NIST Webbook
tb	502.64	K	Joback Method
tc	730.51	K	Joback Method
tf	325.05	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.93	J/mol×K	502.64	Joback Method
cpg	359.43	J/mol×K	540.62	Joback Method
cpg	380.61	J/mol×K	578.60	Joback Method
cpg	400.53	J/mol×K	616.57	Joback Method
cpg	419.22	J/mol×K	654.55	Joback Method
cpg	436.71	J/mol×K	692.53	Joback Method
cpg	453.06	J/mol×K	730.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R120313&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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