

trans-Decahydroquinoline, 10-methyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C10H19N/c1-10-6-3-2-5-9(10)11-8-4-7-10/h9,11H,2-8H2,1H3/t9-,10+/m0/s1

MBQXXEKLNYIWMP-VHSXEESVSA-N

C10H19N

CC12CCCCC1NCCC2

153.26

Physical Properties

Property code	Value	Unit	Source
gf	188.64	kJ/mol	Joback Method
hf	-75.72	kJ/mol	Joback Method
hfus	12.82	kJ/mol	Joback Method
hvap	43.98	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.319		Crippen Method
mcvol	140.020	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	1220.00		NIST Webbook
tb	507.55	K	Joback Method
tc	745.69	K	Joback Method
tf	353.19	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.76	J/mol×K	507.55	Joback Method
cpg	358.90	J/mol×K	547.24	Joback Method
cpg	379.44	J/mol×K	586.93	Joback Method
cpg	398.56	J/mol×K	626.62	Joback Method
cpg	416.43	J/mol×K	666.31	Joback Method
cpg	433.21	J/mol×K	706.00	Joback Method
cpg	449.08	J/mol×K	745.69	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R120368&Units=SI

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

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