DL-trans-Decahydroquinoline

Inchi: InChI=1S/C9H17N/c1-2-6-9-8(4-1)5-3-7-10-9/h8-10H,1-7H2/t8-,9+/m1/s1
InchiKey: POTIYWUALSJREP-BDAKNGLRSA-N
Formula: C9H17N
SMILES: C1CCC2NCCCC2C1
Mol. weight [g/mol]: 139.24
CAS: 105728-23-2

Physical Properties

Property code	Value	Unit	Source
chl	-5780.30 ± 1.20	kJ/mol	NIST Webbook
gf	185.71	kJ/mol	Joback Method
hf	-70.32	kJ/mol	Joback Method
hfl	-190.80 ± 1.40	kJ/mol	NIST Webbook
hfus	16.53	kJ/mol	Joback Method
hvap	53.28	kJ/mol	NIST Webbook
log10ws	-2.44		Crippen Method
logp	1.929		Crippen Method
mcvol	125.930	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
tb	484.43	K	Joback Method
tc	716.50	K	Joback Method
tf	318.02	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.06	J/mol×K	484.43	Joback Method
cpg	310.41	J/mol×K	523.11	Joback Method
cpg	330.45	J/mol×K	561.79	Joback Method
cpg	349.23	J/mol×K	600.46	Joback Method
cpg	366.80	J/mol×K	639.14	Joback Method
cpg	383.22	J/mol×K	677.82	Joback Method
cpg	398.52	J/mol×K	716.50	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=C105728232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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