

1,1-Diethyl-1,2,3,4-tetrahydronaphthalene

Other names:	Naphthalene, 1,1-diethyl-1,2,3,4-tetrahydro
Inchi:	InChI=1S/C14H20/c1-3-14(4-2)11-7-9-12-8-5-6-10-13(12)14/h5-6,8,10H,3-4,7,9,11H2,1-2H
InchiKey:	DBFQMDNLSBZPMF-UHFFFAOYSA-N
Formula:	C14H20
SMILES:	CCC1(CC)CCCc2ccccc21
Mol. weight [g/mol]:	188.31
CAS:	2938-66-1

Physical Properties

Property code	Value	Unit	Source
gf	212.94	kJ/mol	Joback Method
hf	-25.35	kJ/mol	Joback Method
hfus	15.40	kJ/mol	Joback Method
hvap	48.63	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.081		Crippen Method
mcvol	173.500	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	1439.00		NIST Webbook
tb	562.63	K	Joback Method
tc	788.19	K	Joback Method
tf	324.80	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.92	J/molxK	562.63	Joback Method
cpg	448.54	J/molxK	600.22	Joback Method
cpg	466.85	J/molxK	637.82	Joback Method
cpg	484.00	J/molxK	675.41	Joback Method
cpg	500.17	J/molxK	713.00	Joback Method
cpg	515.53	J/molxK	750.59	Joback Method
cpg	530.23	J/molxK	788.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2938661&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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