

4a(2H)-Naphthalenol,1,3,4,7,8,8a-hexahydro-8a-m

Inchi:	InChI=1S/C11H18O/c1-10-6-2-4-8-11(10,12)9-5-3-7-10/h4,8,12H,2-3,5-7,9H2,1H3/t10-,1
InchiKey:	QVIKSWDNWOGDDS-QWRGUYRKSA-N
Formula:	C11H18O
SMILES:	CC12CCC=CC1(O)CCCC2
Mol. weight [g/mol]:	166.26
CAS:	68211-44-9

Physical Properties

Property code	Value	Unit	Source
gf	-3.00	kJ/mol	Joback Method
hf	-213.38	kJ/mol	Joback Method
hfus	4.83	kJ/mol	Joback Method
hvap	55.26	kJ/mol	Joback Method
ie	9.26 ± 0.02	eV	NIST Webbook
log10ws	-3.20		Crippen Method
logp	2.648		Crippen Method
mcvol	145.700	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	573.46	K	Joback Method
tc	795.35	K	Joback Method
tf	344.91	K	Joback Method
vc	0.534	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.33	J/molxK	573.46	Joback Method
cpg	400.36	J/molxK	610.44	Joback Method
cpg	416.21	J/molxK	647.42	Joback Method
cpg	431.12	J/molxK	684.40	Joback Method
cpg	445.35	J/molxK	721.39	Joback Method
cpg	459.13	J/molxK	758.37	Joback Method
cpg	472.71	J/molxK	795.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68211449&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ie:	Ionization energy
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

Latest version available from:

<https://www.cheméo.com/cid/55-617-6/4a-2H-Naphthalenol-1-3-4-7-8-8a-hexahydro-8a-methyl-cis.pdf>

Generated by Cheméo on 2024-04-27 09:10:21.188971069 +0000 UTC m=+16498270.109548390.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.