

Norlevorphanol

Other names:	Morphinan-3-ol Morphinan, 3-hydroxy- (-)-3-Hydroxymorphinan 3-Hydroxymorphinan NIH-7539
Inchi:	InChI=1S/C16H21NO/c18-12-5-4-11-9-15-13-3-1-2-6-16(13,7-8-17-15)14(11)10-12/h4-5,
InchiKey:	IYNWSQDZXMGGGI-UHFFFAOYSA-N
Formula:	C16H21NO
SMILES:	Oc1ccc2c(c1)C13CCCCC1C(C2)NCC3
Mol. weight [g/mol]:	243.34
CAS:	1531-12-0

Physical Properties

Property code	Value	Unit	Source
gf	272.27	kJ/mol	Joback Method
hf	-66.69	kJ/mol	Joback Method
hfus	30.13	kJ/mol	Joback Method
hvap	72.85	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.738		Crippen Method
mcvol	195.810	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2237.00		NIST Webbook
rinpol	2237.00		NIST Webbook
tb	755.31	K	Joback Method
tc	1022.43	K	Joback Method
tf	596.45	K	Joback Method
vc	0.679	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.41	J/molxK	755.31	Joback Method

cpg	636.72	J/mol×K	799.83	Joback Method
cpg	656.44	J/mol×K	844.35	Joback Method
cpg	676.00	J/mol×K	888.87	Joback Method
cpg	695.83	J/mol×K	933.39	Joback Method
cpg	716.37	J/mol×K	977.91	Joback Method
cpg	738.05	J/mol×K	1022.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1531120&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

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

Latest version available from:

<https://www.chemeo.com/cid/92-594-1/Norlevorphanol.pdf>

Generated by Cheméo on 2024-04-19 20:05:50.917187914 +0000 UTC m=+15846399.837765230.

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