

Normorphine

Other names:	Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-, (5«alpha»,6«alpha»)- Demethylmorphine Desmethylmorphine Morphinan-3,6«alpha»-diol, 7,8-didehydro-4,5«alpha»-epoxy- N-Normorphine 4,5-Epoxy-3,6-dihydroxymorphin-7-ene
Inchi:	InChI=1S/C16H17NO3/c18-11-3-1-8-7-10-9-2-4-12(19)15-16(9,5-6-17-10)13(8)14(11)20
InchiKey:	ONBWJWYUHXVEJS-UHFFFAOYSA-N
Formula:	C16H17NO3
SMILES:	Oc1ccc2c3c1OC1C(O)C=CC4C(C2)NCCC341
Mol. weight [g/mol]:	271.31
CAS:	466-97-7

Physical Properties

Property code	Value	Unit	Source
gf	146.90	kJ/mol	Joback Method
hf	-239.83	kJ/mol	Joback Method
hfus	46.43	kJ/mol	Joback Method
hvap	94.26	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	0.856		Crippen Method
mcvol	192.390	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook
tb	872.11	K	Joback Method
tc	1116.32	K	Joback Method
tf	717.86	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	656.81	J/mol×K	872.11	Joback Method
cpg	673.90	J/mol×K	912.81	Joback Method
cpg	691.78	J/mol×K	953.51	Joback Method
cpg	710.83	J/mol×K	994.22	Joback Method
cpg	731.41	J/mol×K	1034.92	Joback Method
cpg	753.91	J/mol×K	1075.62	Joback Method
cpg	778.70	J/mol×K	1116.32	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C466977&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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