

Norcodeine

Other names:	Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-, (5«alpha»,6«alpha»)-Morphinan-6«alpha»-ol, 7,8-didehydro-4,5«alpha»-epoxy-3-methoxy-N-Demethylated codeine N-Desmethylnorcodeine N-Norcodeine Normorphine 3-methyl ether 7,8-Didehydro-4,5-«alpha»-epoxy-3-methoxymorphinan-6-«alpha»-ol N-Demethylcodeine (5«alpha»,6«alpha»)-7,8-Didehydro-4,5-epoxy-3-methoxymorphinan-6-ol
Inchi:	InChI=1S/C17H19NO3/c1-20-13-5-2-9-8-11-10-3-4-12(19)16-17(10,6-7-18-11)14(9)15(1)
InchiKey:	HKOIXWVRNLGFOR-UHFFFAOYSA-N
Formula:	C17H19NO3
SMILES:	COc1ccc2c3c1OC1C(O)C=CC4C(C2)NCCC341
Mol. weight [g/mol]:	285.34
CAS:	467-15-2

Physical Properties

Property code	Value	Unit	Source
gf	195.31	kJ/mol	Joback Method
hf	-226.85	kJ/mol	Joback Method
hfus	44.04	kJ/mol	Joback Method
hvap	86.54	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	1.159		Crippen Method
mcvol	206.480	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2382.00		NIST Webbook
rinpol	2388.00		NIST Webbook
rinpol	2388.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	841.77	K	Joback Method
tc	1073.97	K	Joback Method
tf	652.16	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.16	J/mol×K	841.77	Joback Method
cpg	705.05	J/mol×K	880.47	Joback Method
cpg	721.93	J/mol×K	919.17	Joback Method
cpg	739.06	J/mol×K	957.87	Joback Method
cpg	756.69	J/mol×K	996.57	Joback Method
cpg	775.06	J/mol×K	1035.27	Joback Method
cpg	794.44	J/mol×K	1073.97	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=C467152&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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