Morphinan-6-one, 4,5-epoxy-14-hydroxy-3-methoxy-, (5«alpha»)-

Other names: (5«alpha»)-4,5-epoxy-14-hydroxy-3-methoxymorphinan-6-one
Noroxycodone

Inchi: InChI=1S/C17H19NO4/c1-21-11-3-2-9-8-12-17(20)5-4-10(19)15-16(17,6-7-18-12)13(9)14

InchiKey: RIKMCJUNPCRFMW-UHFFFAOYSA-N

Formula: C17H19NO4

SMILES: COc1ccc2c3c1OC1C(=O)CCC4(O)C(C2)NCCC314

Mol. weight [g/mol]: 301.34

CAS: 57664-96-7

Physical Properties

Property code	Value	Unit	Source
gf	44.98	kJ/mol	Joback Method
hf	-386.75	kJ/mol	Joback Method
hfus	34.96	kJ/mol	Joback Method
hvap	89.65	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	0.706		Crippen Method
mcvol	212.350	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	2684.60		NIST Webbook
rinpol	2684.60		NIST Webbook
tb	915.34	K	Joback Method
tc	1161.69	K	Joback Method
tf	747.76	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.04	J/mol×K	915.34	Joback Method
cpg	764.78	J/mol×K	956.40	Joback Method
cpg	787.89	J/mol×K	997.46	Joback Method
cpg	812.77	J/mol×K	1038.51	Joback Method
cpg	839.78	J/mol×K	1079.57	Joback Method

cpg	869.34	J/mol×K	1120.63	Joback Method
cpg	901.81	J/mol×K	1161.69	Joback Method

Sources

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=C57664967&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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