Morphinan, 3-methoxy-

Other names: 3-Methoxymorphinan
Inchi: InChI=1S/C17H23NO/c1-19-13-6-5-12-10-16-14-4-2-3-7-17(14,8-9-18-16)15(12)11-13/h5
InchiKey: ILNSWVUXAPSPEH-UHFFFAOYSA-N
Formula: C17H23NO
SMILES: COc1ccc2c(c1)C13CCCCC1C(C2)NCC3
Mol. weight [g/mol]: 257.37
CAS: 1531-25-5

Physical Properties

Property code	Value	Unit	Source
gf	320.68	kJ/mol	Joback Method
hf	-53.71	kJ/mol	Joback Method
hfus	27.73	kJ/mol	Joback Method
hvap	65.14	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.041		Crippen Method
mcvol	209.900	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	2146.00		NIST Webbook
tb	724.97	K	Joback Method
tc	976.32	K	Joback Method
tf	530.75	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.85	J/mol×K	724.97	Joback Method
cpg	662.66	J/mol×K	766.86	Joback Method
cpg	683.37	J/mol×K	808.75	Joback Method
cpg	703.26	J/mol×K	850.65	Joback Method
cpg	722.61	J/mol×K	892.54	Joback Method
cpg	741.67	J/mol×K	934.43	Joback Method
cpg	760.72	J/mol×K	976.32	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=C1531255&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