Codeine

Other names:	7,8-Didehydro-4,5-epoxy-3-methoxy-17-ethylmorphanan-6-ol (codeine)
	7,8-Didehydro-4,5«alpha»-epoxy-3-methoxy-17-methyl morphinan-6«alpha»-ol
	7,8-Didehydro-4,5Â«alphaÂ»-epoxy-3-methoxy-17-methyl morphinan-6Â«alphaÂ»-ol
	Codeine anhydrous
	Codicept
	Coducept
	Methylmorphine
	Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, (5«alpha»,6«alpha»)-
	Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, (5Â«alphaÂ»,6Â«alphaÂ»)-
	Morphinan-6«alpha»-ol, 7,8-didehydro-4,5«alpha»-epoxy-3-methoxy-17-methyl-
	Morphinan-6Â«alphaÂ»-ol, 7,8-didehydro-4,5Â«alphaÂ»-epoxy-3-methoxy-17-methyl-
	Morphine monomethyl ether
	Morphine, 3-methyl ether
	Norcodeine, N-methyl-
	O3-Methylmorphine
	Oprea1_828621
	l-Codeine
Inchi:	InChI=1S/C18H21NO3/c1-19-8-7-18-11-4-5-13(20)17(18)22-16-14(21-2)6-3-10(15(16)18
InchiKey:	OROGSEYTTFOCAN-UHFFFAOYSA-N
Formula:	C18H21NO3
SMILES:	COc1ccc2c3c1OC1C(O)C=CC4C(C2)N(C)CCC341
Mol. weight [g/mol]:	299.36
CAS:	76-57-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.26		Aqueous Solubility Prediction Method
logp	1.501		Crippen Method
mcvol	220.570	ml/mol	McGowan Method
rinpol	2382.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2377.00		NIST Webbook
rinpol	2387.00		NIST Webbook
rinpol	2403.00		NIST Webbook
rinpol	2373.00		NIST Webbook
rinpol	2410.00		NIST Webbook

rinpol	2376.00	NIST Webbook
rinpol	2380.00	NIST Webbook
rinpol	2385.00	NIST Webbook
rinpol	2474.40	NIST Webbook
rinpol	2376.00	NIST Webbook
rinpol	2348.00	NIST Webbook
rinpol	2355.00	NIST Webbook
rinpol	2348.00	NIST Webbook
rinpol	2360.00	NIST Webbook
rinpol	2375.00	NIST Webbook
rinpol	2391.00	NIST Webbook
rinpol	2376.00	NIST Webbook
rinpol	2353.00	NIST Webbook
rinpol	2356.00	NIST Webbook
rinpol	2363.00	NIST Webbook
rinpol	2376.00	NIST Webbook
rinpol	2375.00	NIST Webbook
rinpol	2376.00	NIST Webbook
rinpol	2348.00	NIST Webbook
rinpol	2355.00	NIST Webbook
rinpol	2400.00	NIST Webbook
rinpol	2380.00	NIST Webbook
rinpol	2360.00	NIST Webbook
rinpol	2360.00	NIST Webbook
rinpol	2365.00	NIST Webbook
rinpol	2376.00	NIST Webbook
rinpol	2360.00	NIST Webbook
rinpol	2385.00	NIST Webbook
rinpol	2376.00	NIST Webbook
rinpol	2376.00	NIST Webbook
rinpol	2385.00	NIST Webbook
rinpol	2377.00	NIST Webbook
rinpol	2373.00	NIST Webbook
rinpol	2474.40	NIST Webbook
rinpol	2353.00	NIST Webbook
ripol	3567.00	NIST Webbook
ripol	3567.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hfust	23.81	kJ/mol	430.30	NIST Webbook
hfust	18.28	kJ/mol	428.20	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76573&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

hfust: Enthalpy of fusion at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices