OXYCOLCHICINE

Other names: Colchicine, oxo-
Oxycolchicine
10,12a-Epoxycolchicine
Inchi: InChI=1S/C22H25NO7/c1-12(24)23-15-7-6-13-10-16(26-2)19(27-3)20(28-4)18(13)21-8-9
InchiKey: YOEMNGTWNPPXCM-UHFFFAOYSA-N
Formula: C22H25NO7
SMILES: COc1cc2c(c(OC)c1OC)C13C=CC(OC)(O1)C(=O)C=C3C(NC(C)=O)CC2
Mol. weight [g/mol]: 415.44

Physical Properties

Property code	Value	Unit	Source
hfus	43.82	kJ/mol	Joback Method
logp	1.797		Crippen Method
mcvol	298.370	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1077.37	J/mol×K	1070.39	Joback Method
cpg	1104.39	J/mol×K	1112.12	Joback Method
cpg	1132.73	J/mol×K	1153.85	Joback Method
cpg	1162.68	J/mol×K	1195.59	Joback Method
cpg	1194.53	J/mol×K	1237.32	Joback Method
cpg	1228.55	J/mol×K	1279.05	Joback Method
cpg	1265.04	J/mol×K	1320.78	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6788029&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume