

Acetimide, N-(6,7,9,10-tetrahydro-1,2,3,10-tetramethoxy-9-oxo-

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
CAS:	6788-02-9

Physical Properties

Property code	Value	Unit	Source
gf	-262.63	kJ/mol	Joback Method
hf	-823.80	kJ/mol	Joback Method
hfus	43.82	kJ/mol	Joback Method
hvap	100.10	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	1.797		Crippen Method
mcvol	298.370	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
tb	1070.39	K	Joback Method
tc	1320.78	K	Joback Method
tf	809.12	K	Joback Method
vc	1.123	m3/kmol	Joback 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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6788029&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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