

Mescaline

Other names:	mescaline hydrochloride
Inchi:	InChI=1S/C11H17NO3/c1-13-9-6-8(4-5-12)7-10(14-2)11(9)15-3/h6-7H,4-5,12H2,1-3H3
InchiKey:	RHCSKNNOAZULRK-UHFFFAOYSA-N
Formula:	C11H17NO3
SMILES:	COc1cc(CCN)cc(OC)c1OC
Mol. weight [g/mol]:	211.26

Physical Properties

Property code	Value	Unit	Source
hfus	25.88	kJ/mol	Joback Method
ie	7.93	eV	Cheméo Relay (1.0)
log10ws	-1.62		Cheméo Relay (1.0)
logp	1.214		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
tf	376.54	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.68	J/mol×K	632.49	Joback Method
cpg	451.89	J/mol×K	667.21	Joback Method
cpg	465.41	J/mol×K	701.93	Joback Method
cpg	478.24	J/mol×K	736.65	Joback Method
cpg	490.35	J/mol×K	771.37	Joback Method
cpg	501.72	J/mol×K	806.09	Joback Method
cpg	512.33	J/mol×K	840.81	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=C54046&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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