Halazepam M (desalkylhydroxymethoxy-), hydrolysis, acetylated

Inchi: InChI=1S/C18H16ClNO5/c1-10(21)20-16-7-4-12(19)8-15(16)18(23)14-6-5-13(25-11(2)22

InchiKey: YAVGBOLTWPWPTQ-UHFFFAOYSA-N

Formula: C18H16ClNO5

SMILES: COc1cc(OC(C)=O)ccc1C(=O)c1cc(Cl)ccc1NC(C)=O

Mol. weight [g/mol]: 361.78

Physical Properties

Property code	Value	Unit	Source
hfus	45.37	kJ/mol	Joback Method
ie	7.77	eV	Cheméo Relay (1.0)
logp	3.463		Crippen Method
mcvol	255.630	ml/mol	McGowan Method
rinpol	2990.00		NIST Webbook
rinpol	2990.00		NIST Webbook
rinpol	2990.00		NIST Webbook
tb	685.17	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.03	J/mol×K	978.57	Joback Method
cpg	751.93	J/mol×K	1018.59	Joback Method
cpg	759.46	J/mol×K	1058.61	Joback Method
cpg	765.64	J/mol×K	1098.62	Joback Method
cpg	770.48	J/mol×K	1138.64	Joback Method
cpg	773.99	J/mol×K	1178.66	Joback Method
cpg	776.20	J/mol×K	1218.68	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312933&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature