Halazepam M (hydroxymethoxy-), hydrolysis, acetylated

Inchi: InChI=1S/C20H17ClF3NO5/c1-11(26)25(10-20(22,23)24)17-7-4-13(21)8-16(17)19(28)15

InchiKey: DPXXVSWQVAHFIH-UHFFFAOYSA-N

Formula: C20H17ClF3NO5

SMILES: COc1cc(OC(C)=O)ccc1C(=O)c1cc(Cl)ccc1N(CC(F)(F)F)C(C)=O

Mol. weight [g/mol]: 443.80

Physical Properties

Property code	Value	Unit	Source
gf	-775.68	kJ/mol	Joback Method
hf	-1176.42	kJ/mol	Joback Method
hfus	50.30	kJ/mol	Joback Method
hvap	95.05	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.420		Crippen Method
mcvol	289.120	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	2500.00		NIST Webbook
tb	981.18	K	Joback Method
tc	1208.76	K	Joback Method
tf	678.91	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.11	J/mol×K	981.18	Joback Method
cpg	879.61	J/mol×K	1019.11	Joback Method
cpg	887.98	J/mol×K	1057.04	Joback Method
cpg	895.27	J/mol×K	1094.97	Joback Method
cpg	901.55	J/mol×K	1132.90	Joback Method
cpg	906.86	J/mol×K	1170.83	Joback Method
cpg	911.26	J/mol×K	1208.76	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313154&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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