Halazepam M (hydroxy-), isomer 1, hydrolysis, acetylated

Inchi: InChI=1S/C19H15ClF3NO4/c1-11(25)24(10-19(21,22)23)17-8-5-14(20)9-16(17)18(27)13

InchiKey: RDVTXNNIRLUHCM-UHFFFAOYSA-N

Formula: C19H15ClF3NO4

SMILES: CC(=O)Oc1ccc(C(=O)c2cc(Cl)ccc2N(CC(F)(F)F)C(C)=O)cc1

Mol. weight [g/mol]: 413.77

Physical Properties

Property code	Value	Unit	Source
gf	-669.47	kJ/mol	Joback Method
hf	-1012.09	kJ/mol	Joback Method
hfus	46.91	kJ/mol	Joback Method
hvap	89.75	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.411		Crippen Method
mcvol	269.160	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		NIST Webbook
tb	930.90	K	Joback Method
tc	1156.29	K	Joback Method
tf	632.89	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.09	J/mol×K	930.90	Joback Method
cpg	800.20	J/mol×K	968.46	Joback Method
cpg	809.32	J/mol×K	1006.03	Joback Method
cpg	817.54	J/mol×K	1043.59	Joback Method
cpg	824.94	J/mol×K	1081.16	Joback Method
cpg	831.58	J/mol×K	1118.72	Joback Method
cpg	837.56	J/mol×K	1156.29	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=R313134&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