Halazepam, hydrolysis

Inchi: InChI=1S/C18H15ClF3NO2/c1-12(24)23(10-9-18(20,21)22)16-8-7-14(19)11-15(16)17(25
InchiKey: JJSNDXZGTNQKCR-UHFFFAOYSA-N
Formula: C18H15ClF3NO2
SMILES: CC(=O)N(CCC(F)(F)F)c1ccc(Cl)cc1C(=O)c1ccccc1
Mol. weight [g/mol]: 369.76

Physical Properties

Property code	Value	Unit	Source
gf	-434.34	kJ/mol	Joback Method
hf	-735.18	kJ/mol	Joback Method
hfus	41.92	kJ/mol	Joback Method
hvap	77.71	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.876		Crippen Method
mcvol	247.630	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook
tb	826.75	K	Joback Method
tc	1046.81	K	Joback Method
tf	536.94	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.20	J/mol×K	826.75	Joback Method
cpg	714.40	J/mol×K	863.43	Joback Method
cpg	725.60	J/mol×K	900.10	Joback Method
cpg	735.91	J/mol×K	936.78	Joback Method
cpg	745.42	J/mol×K	973.46	Joback Method
cpg	754.22	J/mol×K	1010.13	Joback Method
cpg	762.41	J/mol×K	1046.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313085&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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