Ethylloflazepate, hydrolysis, acetylated

Inchi: InChI=1S/C15H11ClFNO2/c1-9(19)18-14-7-6-10(16)8-12(14)15(20)11-4-2-3-5-13(11)17/
InchiKey: BIJCUDKFSIRCDI-UHFFFAOYSA-N
Formula: C15H11ClFNO2
SMILES: CC(=O)Nc1ccc(Cl)cc1C(=O)c1ccccc1F
Mol. weight [g/mol]: 291.70

Physical Properties

Property code	Value	Unit	Source
gf	-103.84	kJ/mol	Joback Method
hf	-297.82	kJ/mol	Joback Method
hfus	37.09	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.668		Crippen Method
mcvol	201.820	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	805.51	K	Joback Method
tc	1043.82	K	Joback Method
tf	532.24	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.69	J/mol×K	805.51	Joback Method
cpg	542.86	J/mol×K	845.23	Joback Method
cpg	553.02	J/mol×K	884.95	Joback Method
cpg	562.23	J/mol×K	924.67	Joback Method
cpg	570.55	J/mol×K	964.39	Joback Method

cpg	578.03	J/mol×K	1004.10	Joback Method
cpg	584.72	J/mol×K	1043.82	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=R313005&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