FLUNIXIN METHYL ESTER

Other names: Flunixin methyl derivative
Flunixin, methyl deriv.
Inchi: InChI=1S/C15H13F3N2O2/c1-9-11(15(16,17)18)6-3-7-12(9)20-13-10(14(21)22-2)5-4-8-1
InchiKey: YKASBHLSNBJQJF-UHFFFAOYSA-N
Formula: C15H13F3N2O2
SMILES: COC(=O)c1cccnc1Nc1cccc(C(F)(F)F)c1C
Mol. weight [g/mol]: 310.27

Physical Properties

Property code	Value	Unit	Source
hvap	92.31	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.72		Cheméo Relay (1.0)
logp	3.939		Crippen Method
mcvol	207.400	ml/mol	McGowan Method
tf	397.11	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C75369630&Units=SI
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
Cheméo Relay (1.0):

Legend

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

tf: Normal melting (fusion) point