

Celecoxib

Other names:	Celebrex 4-[5-(3-Methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]-benzenesulphonamide (celecoxib)
Inchi:	InChI=1S/C17H14F3N3O2S/c1-11-2-4-12(5-3-11)15-10-16(17(18,19)20)22-23(15)13-6-8
InchiKey:	RZEKVGVHFLEQIL-UHFFFAOYSA-N
Formula:	C17H14F3N3O2S
SMILES:	<chem>Cc1ccc(-c2cc(C(F)(F)F)nn2-c2ccc(S(N)(=O)=O)cc2)cc1</chem>
Mol. weight [g/mol]:	381.37
CAS:	169590-42-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.77		Crippen Method
logp	3.514		Crippen Method
mcvol	246.750	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	34.35	kJ/mol	436.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C169590425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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