

indoprofen

Inchi:	InChI=1S/C17H15NO3/c1-11(17(20)21)12-6-8-14(9-7-12)18-10-13-4-2-3-5-15(13)16(18)
InchiKey:	RJMIEHBSYVWVIN-UHFFFAOYSA-N
Formula:	C17H15NO3
SMILES:	CC(C(=O)O)c1ccc(N2Cc3ccccc3C2=O)cc1
Mol. weight [g/mol]:	281.31
CAS:	31842-01-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Aqueous Solubility Prediction Method
logp	3.035		Crippen Method
mcvol	211.000	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	40.30	kJ/mol	484.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31842010&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx

Legend

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

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