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/AqueousDa

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