ibuproxam

Inchi: InChI=1S/C13H19NO2/c1-9(2)8-11-4-6-12(7-5-11)10(3)13(15)14-16/h4-7,9-10,16H,8H2,
InchiKey: BYPIURIATSUHDW-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: CC(C)Cc1ccc(C(C)C(=O)NO)cc1
Mol. weight [g/mol]: 221.30

Physical Properties

Property code	Value	Unit	Source
gf	-19.87	kJ/mol	Joback Method
hf	-308.49	kJ/mol	Joback Method
hfus	26.82	kJ/mol	Joback Method
hvap	76.56	kJ/mol	Joback Method
log10ws	-3.04		Aqueous Solubility Prediction Method
logp	2.494		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
tb	723.84	K	Joback Method
tc	925.16	K	Joback Method
tf	408.62	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.45	J/mol×K	723.84	Joback Method
cpg	541.55	J/mol×K	757.39	Joback Method
cpg	553.84	J/mol×K	790.95	Joback Method
cpg	565.34	J/mol×K	824.50	Joback Method
cpg	576.09	J/mol×K	858.05	Joback Method
cpg	586.13	J/mol×K	891.61	Joback Method
cpg	595.49	J/mol×K	925.16	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume