

Ibuprofen, hydroxy, bis-methylated

Inchi:	InChI=1S/C15H22O3/c1-10(2)8-13-7-6-12(9-14(13)17-4)11(3)15(16)18-5/h6-7,9-11H,8H
InchiKey:	COGYHUFQBYMIDH-UHFFFAOYSA-N
Formula:	C15H22O3
SMILES:	<chem>COC(=O)C(C)c1ccc(CC(C)C)c(OC)c1</chem>
Mol. weight [g/mol]:	250.33

Physical Properties

Property code	Value	Unit	Source
gf	-175.23	kJ/mol	Joback Method
hf	-526.92	kJ/mol	Joback Method
hfus	24.80	kJ/mol	Joback Method
hvap	63.37	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.170		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	1680.00		NIST Webbook
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tb	677.07	K	Joback Method
tc	881.74	K	Joback Method
tf	374.66	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.52	J/molxK	677.07	Joback Method
cpg	591.25	J/molxK	711.18	Joback Method
cpg	607.04	J/molxK	745.29	Joback Method
cpg	621.89	J/molxK	779.41	Joback Method
cpg	635.81	J/molxK	813.52	Joback Method
cpg	648.81	J/molxK	847.63	Joback Method
cpg	660.88	J/molxK	881.74	Joback Method
dvisc	0.0012729	Paxs	374.66	Joback Method

dvisc	0.0006305	Paxs	425.06	Joback Method
dvisc	0.0003625	Paxs	475.46	Joback Method
dvisc	0.0002317	Paxs	525.87	Joback Method
dvisc	0.0001602	Paxs	576.27	Joback Method
dvisc	0.0001175	Paxs	626.67	Joback Method
dvisc	0.0000903	Paxs	677.07	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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