

Ibuprofen, isobutyl ester

Inchi:	InChI=1S/C17H26O2/c1-12(2)10-15-6-8-16(9-7-15)14(5)17(18)19-11-13(3)4/h6-9,12-14H
InchiKey:	IZQZIVHKRMBEMV-UHFFFAOYSA-N
Formula:	C17H26O2
SMILES:	CC(C)COC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]:	262.39

Physical Properties

Property code	Value	Unit	Source
gf	-46.20	kJ/mol	Joback Method
hf	-429.79	kJ/mol	Joback Method
hfus	25.66	kJ/mol	Joback Method
hvap	64.37	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.188		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	1428.00		NIST Webbook
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tb	694.99	K	Joback Method
tc	898.84	K	Joback Method
tf	347.45	K	Joback Method
vc	0.885	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.04	J/molxK	694.99	Joback Method
cpg	674.33	J/molxK	728.96	Joback Method
cpg	691.53	J/molxK	762.94	Joback Method
cpg	707.68	J/molxK	796.91	Joback Method
cpg	722.81	J/molxK	830.89	Joback Method
cpg	736.95	J/molxK	864.86	Joback Method
cpg	750.13	J/molxK	898.84	Joback Method
dvisc	0.0026098	Paxs	347.45	Joback Method

dvisc	0.0009827	Paxs	405.37	Joback Method
dvisc	0.0004724	Paxs	463.30	Joback Method
dvisc	0.0002672	Paxs	521.22	Joback Method
dvisc	0.0001694	Paxs	579.14	Joback Method
dvisc	0.0001167	Paxs	637.07	Joback Method
dvisc	0.0000855	Paxs	694.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389599&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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