

Ibuprofen, pentyl ester

Inchi:	InChI=1S/C18H28O2/c1-5-6-7-12-20-18(19)15(4)17-10-8-16(9-11-17)13-14(2)3/h8-11,14
InchiKey:	HIIBDGSTBGJOBG-UHFFFAOYSA-N
Formula:	C18H28O2
SMILES:	CCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]:	276.41

Physical Properties

Property code	Value	Unit	Source
gf	-35.34	kJ/mol	Joback Method
hf	-445.15	kJ/mol	Joback Method
hfus	31.77	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.722		Crippen Method
mvol	248.160	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
tb	718.31	K	Joback Method
tc	916.84	K	Joback Method
tf	373.72	K	Joback Method
vc	0.948	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.65	J/molxK	718.31	Joback Method
cpg	729.87	J/molxK	751.40	Joback Method
cpg	747.03	J/molxK	784.49	Joback Method
cpg	763.16	J/molxK	817.57	Joback Method
cpg	778.29	J/molxK	850.66	Joback Method
cpg	792.46	J/molxK	883.75	Joback Method
cpg	805.69	J/molxK	916.84	Joback Method
dvisc	0.0018526	Paxs	373.72	Joback Method

dvisc	0.0007788	Paxs	431.15	Joback Method
dvisc	0.0004014	Paxs	488.58	Joback Method
dvisc	0.0002378	Paxs	546.02	Joback Method
dvisc	0.0001557	Paxs	603.45	Joback Method
dvisc	0.0001097	Paxs	660.88	Joback Method
dvisc	0.0000817	Paxs	718.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390161&Units=SI

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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