

Ibuprofen, undecyl ester

Inchi:	InChI=1S/C24H40O2/c1-5-6-7-8-9-10-11-12-13-18-26-24(25)21(4)23-16-14-22(15-17-23
InchiKey:	NAVARDVMHVYAAF-UHFFFAOYSA-N
Formula:	C24H40O2
SMILES:	CCCCCCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]:	360.57

Physical Properties

Property code	Value	Unit	Source
gf	15.18	kJ/mol	Joback Method
hf	-568.99	kJ/mol	Joback Method
hfus	47.31	kJ/mol	Joback Method
hvap	80.34	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	7.063		Crippen Method
mcvol	332.700	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	1810.00		NIST Webbook
rinpol	1810.00		NIST Webbook
tb	855.59	K	Joback Method
tc	1053.66	K	Joback Method
tf	441.34	K	Joback Method
vc	1.284	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.48	J/molxK	855.59	Joback Method
cpg	1153.65	J/molxK	1020.65	Joback Method
cpg	1138.89	J/molxK	987.64	Joback Method
cpg	1123.03	J/molxK	954.62	Joback Method
cpg	1106.04	J/molxK	921.61	Joback Method
cpg	1087.88	J/molxK	888.60	Joback Method
cpg	1167.37	J/molxK	1053.66	Joback Method
dvisc	0.0000363	Paxs	855.59	Joback Method

dvisc	0.0000494	Paxs	786.55	Joback Method
dvisc	0.0000713	Paxs	717.51	Joback Method
dvisc	0.0001112	Paxs	648.46	Joback Method
dvisc	0.0001928	Paxs	579.42	Joback Method
dvisc	0.0003880	Paxs	510.38	Joback Method
dvisc	0.0009721	Paxs	441.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U390445&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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