

Ibuprofen, decyl ester

Inchi:	InChI=1S/C23H38O2/c1-5-6-7-8-9-10-11-12-17-25-23(24)20(4)22-15-13-21(14-16-22)18
InchiKey:	UPSCHJQYUMXKRL-UHFFFAOYSA-N
Formula:	C23H38O2
SMILES:	CCCCCCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]:	346.55

Physical Properties

Property code	Value	Unit	Source
gf	6.76	kJ/mol	Joback Method
hf	-548.35	kJ/mol	Joback Method
hfus	44.72	kJ/mol	Joback Method
hvap	78.11	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	6.672		Crippen Method
mvol	318.610	ml/mol	McGowan Method
pc	1076.39	kPa	Joback Method
rinpol	1765.00		NIST Webbook
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tb	832.71	K	Joback Method
tc	1029.25	K	Joback Method
tf	430.07	K	Joback Method
vc	1.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.95	J/molxK	832.71	Joback Method
cpg	1091.44	J/molxK	996.49	Joback Method
cpg	1076.75	J/molxK	963.74	Joback Method
cpg	1061.00	J/molxK	930.98	Joback Method
cpg	1044.14	J/molxK	898.22	Joback Method
cpg	1026.14	J/molxK	865.47	Joback Method
cpg	1105.11	J/molxK	1029.25	Joback Method
dvisc	0.0000419	Paxs	832.71	Joback Method

dvisc	0.0000568	Paxs	765.60	Joback Method
dvisc	0.0000818	Paxs	698.50	Joback Method
dvisc	0.0001272	Paxs	631.39	Joback Method
dvisc	0.0002198	Paxs	564.28	Joback Method
dvisc	0.0004401	Paxs	497.18	Joback Method
dvisc	0.0010942	Paxs	430.07	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=U390444&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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