

Ibuprofen, octadecyl ester

Inchi:	InChI=1S/C31H54O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-25-33-31(32)28(4
InchiKey:	YTYVKCLBZWBXLO-UHFFFAOYSA-N
Formula:	C31H54O2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]:	458.76

Physical Properties

Property code	Value	Unit	Source
gf	74.12	kJ/mol	Joback Method
hf	-713.47	kJ/mol	Joback Method
hfus	65.44	kJ/mol	Joback Method
hvap	95.92	kJ/mol	Joback Method
log10ws	-10.45		Crippen Method
logp	9.793		Crippen Method
mcvol	431.330	ml/mol	McGowan Method
pc	686.73	kPa	Joback Method
rinpol	2407.00		NIST Webbook
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tb	1015.75	K	Joback Method
tc	1249.65	K	Joback Method
tf	520.23	K	Joback Method
vc	1.675	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1515.05	J/molxK	1015.75	Joback Method
cpg	1536.95	J/molxK	1054.73	Joback Method
cpg	1557.10	J/molxK	1093.72	Joback Method
cpg	1575.62	J/molxK	1132.70	Joback Method
cpg	1592.59	J/molxK	1171.69	Joback Method
cpg	1608.13	J/molxK	1210.67	Joback Method
cpg	1622.34	J/molxK	1249.65	Joback Method
dvisc	0.0003894	Paxs	520.23	Joback Method

dvisc	0.0001487	Paxs	602.82	Joback Method
dvisc	0.0000716	Paxs	685.40	Joback Method
dvisc	0.0000404	Paxs	767.99	Joback Method
dvisc	0.0000254	Paxs	850.58	Joback Method
dvisc	0.0000174	Paxs	933.16	Joback Method
dvisc	0.0000126	Paxs	1015.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390452&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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