

Ibuprofen, tridecyl ester

Inchi:	InChI=1S/C26H44O2/c1-5-6-7-8-9-10-11-12-13-14-15-20-28-26(27)23(4)25-18-16-24(17)
InchiKey:	AYEGXDMHSIEBT-UHFFFAOYSA-N
Formula:	C26H44O2
SMILES:	CCCCCCCCCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]:	388.63

Physical Properties

Property code	Value	Unit	Source
gf	32.02	kJ/mol	Joback Method
hf	-610.27	kJ/mol	Joback Method
hfus	52.49	kJ/mol	Joback Method
hvap	84.79	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	7.843		Crippen Method
mcvol	360.880	ml/mol	McGowan Method
pc	898.56	kPa	Joback Method
rinsol	1932.00		NIST Webbook
tb	901.35	K	Joback Method
tc	1104.84	K	Joback Method
tf	463.88	K	Joback Method
vc	1.395	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1193.51	J/molxK	901.35	Joback Method
cpg	1213.39	J/molxK	935.26	Joback Method
cpg	1231.96	J/molxK	969.18	Joback Method
cpg	1249.25	J/molxK	1003.09	Joback Method
cpg	1265.33	J/molxK	1037.01	Joback Method
cpg	1280.25	J/molxK	1070.92	Joback Method
cpg	1294.07	J/molxK	1104.84	Joback Method
dvisc	0.0007594	Paxs	463.88	Joback Method
dvisc	0.0002989	Paxs	536.79	Joback Method

dvisc	0.0001470	Paxs	609.70	Joback Method
dvisc	0.0000841	Paxs	682.62	Joback Method
dvisc	0.0000536	Paxs	755.53	Joback Method
dvisc	0.0000370	Paxs	828.44	Joback Method
dvisc	0.0000271	Paxs	901.35	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=U390447&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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