

Naproxen, hydroxy, bis-methylated

Inchi:	InChI=1S/C16H18O4/c1-10(16(17)20-4)11-5-7-13-12(9-11)6-8-14(18-2)15(13)19-3/h5-10
InchiKey:	MXDKTYZSLFNANP-UHFFFAOYSA-N
Formula:	C16H18O4
SMILES:	<chem>COC(=O)C(C)c1ccc2c(OC)c(OC)ccc2c1</chem>
Mol. weight [g/mol]:	274.31

Physical Properties

Property code	Value	Unit	Source
gf	-172.35	kJ/mol	Joback Method
hf	-494.90	kJ/mol	Joback Method
hfus	28.73	kJ/mol	Joback Method
hvap	70.70	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.134		Crippen Method
mvol	212.260	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook
tb	746.77	K	Joback Method
tc	965.81	K	Joback Method
tf	468.38	K	Joback Method
vc	0.799	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.20	J/molxK	746.77	Joback Method
cpg	603.99	J/molxK	783.28	Joback Method
cpg	617.77	J/molxK	819.78	Joback Method
cpg	630.55	J/molxK	856.29	Joback Method
cpg	642.35	J/molxK	892.79	Joback Method
cpg	653.17	J/molxK	929.30	Joback Method
cpg	663.04	J/molxK	965.81	Joback Method
dvisc	0.0006366	Paxs	468.38	Joback Method

dvisc	0.0004292	Paxs	514.78	Joback Method
dvisc	0.0003088	Paxs	561.18	Joback Method
dvisc	0.0002336	Paxs	607.58	Joback Method
dvisc	0.0001839	Paxs	653.97	Joback Method
dvisc	0.0001494	Paxs	700.37	Joback Method
dvisc	0.0001246	Paxs	746.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201808&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

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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