

Fenoprofen, methylated

Inchi:	InChI=1S/C16H16O3/c1-12(16(17)18-2)13-7-6-10-15(11-13)19-14-8-4-3-5-9-14/h3-12H,1
InchiKey:	FUOQIQZCJJDBGD-UHFFFAOYSA-N
Formula:	C16H16O3
SMILES:	<chem>COC(=O)C(C)c1cccc(Oc2ccccc2)c1</chem>
Mol. weight [g/mol]:	256.30
CAS:	66202-87-7

Physical Properties

Property code	Value	Unit	Source
gf	-42.33	kJ/mol	Joback Method
hf	-294.28	kJ/mol	Joback Method
hfus	25.34	kJ/mol	Joback Method
hvap	67.60	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.755		Crippen Method
mcvol	202.090	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	1970.00		NIST Webbook
tb	722.09	K	Joback Method
tc	957.04	K	Joback Method
tf	414.83	K	Joback Method
vc	0.751	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.99	J/molxK	722.09	Joback Method
cpg	611.82	J/molxK	917.88	Joback Method
cpg	600.83	J/molxK	878.72	Joback Method
cpg	588.68	J/molxK	839.56	Joback Method
cpg	575.35	J/molxK	800.41	Joback Method
cpg	560.79	J/molxK	761.25	Joback Method
cpg	621.69	J/molxK	957.04	Joback Method
dvisc	0.0000877	Paxs	722.09	Joback Method

dvisc	0.0001126	Paxs	670.88	Joback Method
dvisc	0.0001506	Paxs	619.67	Joback Method
dvisc	0.0002123	Paxs	568.46	Joback Method
dvisc	0.0003202	Paxs	517.25	Joback Method
dvisc	0.0005287	Paxs	466.04	Joback Method
dvisc	0.0009881	Paxs	414.83	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=C66202877&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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