

Ketoprofen methyl ester

Other names:	Ketoprofen methyl derivative Ketoprofen, methylated
Inchi:	InChI=1S/C17H16O3/c1-12(17(19)20-2)14-9-6-10-15(11-14)16(18)13-7-4-3-5-8-13/h3-12
InchiKey:	BIOCOYIPJQMGTN-UHFFFAOYSA-N
Formula:	C17H16O3
SMILES:	<chem>COC(=O)C(C)c1cccc(C(=O)c2ccccc2)c1</chem>
Mol. weight [g/mol]:	268.31
CAS:	47087-07-0

Physical Properties

Property code	Value	Unit	Source
gf	-57.83	kJ/mol	Joback Method
hf	-295.28	kJ/mol	Joback Method
hfus	28.34	kJ/mol	Joback Method
hvap	74.16	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.194		Crippen Method
mvol	211.880	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	2090.00		NIST Webbook
tb	776.42	K	Joback Method
tc	1015.41	K	Joback Method
tf	453.80	K	Joback Method
vc	0.795	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.17	J/mol×K	776.42	Joback Method
cpg	601.73	J/mol×K	816.25	Joback Method
cpg	615.02	J/mol×K	856.08	Joback Method
cpg	627.11	J/mol×K	895.91	Joback Method
cpg	638.03	J/mol×K	935.74	Joback Method
cpg	647.86	J/mol×K	975.58	Joback Method

cpg	656.63	J/molxK	1015.41	Joback Method
dvisc	0.0010641	Paxs	453.80	Joback Method
dvisc	0.0005828	Paxs	507.57	Joback Method
dvisc	0.0003582	Paxs	561.34	Joback Method
dvisc	0.0002397	Paxs	615.11	Joback Method
dvisc	0.0001711	Paxs	668.88	Joback Method
dvisc	0.0001284	Paxs	722.65	Joback Method
dvisc	0.0001003	Paxs	776.42	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=C47087070&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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