KETOPROFEN ME-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: COC(=O)C(C)c1cccc(C(=O)c2ccccc2)c1
Mol. weight [g/mol]: 268.31

Physical Properties

Property code	Value	Unit	Source
af	0.6340		Cheméo Relay (1.0)
hf	-357.58	kJ/mol	Cheméo Relay (1.0)
hfus	28.34	kJ/mol	Joback Method
hvap	102.45	kJ/mol	Cheméo Relay (1.0)
ie	8.91	eV	Cheméo Relay (1.0)
log10ws	-3.82		Cheméo Relay (1.0)
logp	3.194		Crippen Method
mcvol	211.880	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	2090.00		NIST Webbook
tb	625.21	K	Cheméo Relay (1.0)
tc	877.51	K	Cheméo Relay (1.0)
tf	325.52	K	Cheméo Relay (1.0)
vc	0.754	m3/kmol	Cheméo Relay (1.0)

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/mol×K	1015.41	Joback Method
dvisc	0.0010641	Pa×s	453.80	Joback Method
dvisc	0.0005828	Pa×s	507.57	Joback Method
dvisc	0.0003582	Pa×s	561.34	Joback Method
dvisc	0.0002397	Pa×s	615.11	Joback Method
dvisc	0.0001711	Pa×s	668.88	Joback Method
dvisc	0.0001284	Pa×s	722.65	Joback Method
dvisc	0.0001003	Pa×s	776.42	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C47087070&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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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