1-(4-Methoxyphenyl)prop-2-en-1-one

Inchi: InChI=1S/C10H10O2/c1-3-10(11)8-4-6-9(12-2)7-5-8/h3-7H,1H2,2H3
InchiKey: YMESWDPSFKMFND-UHFFFAOYSA-N
Formula: C10H10O2
SMILES: C=CC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 162.19
CAS: 7448-86-4

Physical Properties

Property code	Value	Unit	Source
gf	-9.98	kJ/mol	Joback Method
hf	-144.04	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	49.28	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.064		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	1452.70		NIST Webbook
rinpol	1452.70		NIST Webbook
tb	532.83	K	Joback Method
tc	751.29	K	Joback Method
tf	311.80	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.47	J/mol×K	532.83	Joback Method
cpg	294.02	J/mol×K	569.24	Joback Method
cpg	305.84	J/mol×K	605.65	Joback Method
cpg	316.97	J/mol×K	642.06	Joback Method
cpg	327.40	J/mol×K	678.47	Joback Method
cpg	337.18	J/mol×K	714.88	Joback Method
cpg	346.30	J/mol×K	751.29	Joback Method

dvisc	0.0016570	Pa×s	311.80	Joback Method
dvisc	0.0009841	Pa×s	348.64	Joback Method
dvisc	0.0006457	Pa×s	385.48	Joback Method
dvisc	0.0004560	Pa×s	422.31	Joback Method
dvisc	0.0003405	Pa×s	459.15	Joback Method
dvisc	0.0002655	Pa×s	495.99	Joback Method
dvisc	0.0002143	Pa×s	532.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C7448864&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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