

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7448864&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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