3-Buten-2-one, 4-(2-methoxyphenyl)-

Other names: 4-(2-Methoxyphenyl)but-3-en-2-one
Inchi: InChI=1S/C11H12O2/c1-9(12)7-8-10-5-3-4-6-11(10)13-2/h3-8H,1-2H3/b8-7+
InchiKey: BTSZEPMWUWYLCP-BQYQJAHWSA-N
Formula: C11H12O2
SMILES: COc1ccccc1C=CC(C)=O
Mol. weight [g/mol]: 176.21
CAS: 10542-87-7

Physical Properties

Property code	Value	Unit	Source
gf	-9.18	kJ/mol	Joback Method
hf	-172.89	kJ/mol	Joback Method
hfus	20.89	kJ/mol	Joback Method
hvap	52.13	kJ/mol	Joback Method
ie	8.20 ± 0.10	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
log10ws	-2.53		Crippen Method
logp	2.297		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
tb	563.19	K	Joback Method
tc	783.00	K	Joback Method
tf	319.75	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.84	J/mol×K	563.19	Joback Method
cpg	340.44	J/mol×K	599.82	Joback Method
cpg	353.23	J/mol×K	636.46	Joback Method
cpg	365.23	J/mol×K	673.09	Joback Method
cpg	376.46	J/mol×K	709.73	Joback Method
cpg	386.97	J/mol×K	746.36	Joback Method

cpg	396.77	J/mol×K	783.00	Joback Method
dvisc	0.0015957	Pa×s	319.75	Joback Method
dvisc	0.0008853	Pa×s	360.32	Joback Method
dvisc	0.0005534	Pa×s	400.90	Joback Method
dvisc	0.0003771	Pa×s	441.47	Joback Method
dvisc	0.0002741	Pa×s	482.04	Joback Method
dvisc	0.0002094	Pa×s	522.62	Joback Method
dvisc	0.0001663	Pa×s	563.19	Joback Method

Sources

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=C10542877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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