3-Penten-2-one, 4-methoxy-3-methyl-, (Z)-

Inchi: InChI=1S/C7H12O2/c1-5(6(2)8)7(3)9-4/h1-4H3/b7-5+
InchiKey: RMUYPYQKKMMBSQ-FNORWQNLSA-N
Formula: C7H12O2
SMILES: COC(C)=C(C)C(C)=O
Mol. weight [g/mol]: 128.17
CAS: 82481-18-3

Physical Properties

Property code	Value	Unit	Source
gf	-162.74	kJ/mol	Joback Method
hf	-334.97	kJ/mol	Joback Method
hfus	14.26	kJ/mol	Joback Method
hvap	40.45	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	439.77	K	Joback Method
tc	632.06	K	Joback Method
tf	207.81	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.56	J/mol×K	439.77	Joback Method
cpg	233.67	J/mol×K	471.82	Joback Method
cpg	244.30	J/mol×K	503.87	Joback Method
cpg	254.47	J/mol×K	535.92	Joback Method
cpg	264.18	J/mol×K	567.96	Joback Method
cpg	273.46	J/mol×K	600.01	Joback Method
cpg	282.30	J/mol×K	632.06	Joback Method

Sources

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=C82481183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume