6-(4-Methoxyphenyl)hex-3-en-2-one

Inchi: InChI=1S/C13H16O2/c1-11(14)5-3-4-6-12-7-9-13(15-2)10-8-12/h3,5,7-10H,4,6H2,1-2H3/
InchiKey: VHCHKVTYZDWNGL-HWKANZROSA-N
Formula: C13H16O2
SMILES: COc1ccc(CCC=CC(C)=O)cc1
Mol. weight [g/mol]: 204.26
CAS: 118790-84-4

Physical Properties

Property code	Value	Unit	Source
gf	7.66	kJ/mol	Joback Method
hf	-214.17	kJ/mol	Joback Method
hfus	26.07	kJ/mol	Joback Method
hvap	56.58	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.773		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	1755.20		NIST Webbook
rinpol	1755.20		NIST Webbook
tb	608.95	K	Joback Method
tc	821.29	K	Joback Method
tf	342.29	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.62	J/mol×K	608.95	Joback Method
cpg	437.68	J/mol×K	644.34	Joback Method
cpg	451.85	J/mol×K	679.73	Joback Method
cpg	465.17	J/mol×K	715.12	Joback Method
cpg	477.67	J/mol×K	750.51	Joback Method
cpg	489.38	J/mol×K	785.90	Joback Method
cpg	500.34	J/mol×K	821.29	Joback Method

dvisc	0.0015261	Pa×s	342.29	Joback Method
dvisc	0.0008169	Pa×s	386.73	Joback Method
dvisc	0.0004975	Pa×s	431.18	Joback Method
dvisc	0.0003323	Pa×s	475.62	Joback Method
dvisc	0.0002379	Pa×s	520.06	Joback Method
dvisc	0.0001795	Pa×s	564.51	Joback Method
dvisc	0.0001411	Pa×s	608.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C118790844&Units=SI
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

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