4-Hexen-3-one, 1-(3,4-methylenedioxyphenyl)

Inchi: InChI=1S/C13H14O3/c1-2-11(14)5-3-4-10-6-7-12-13(8-10)16-9-15-12/h3,5-8H,2,4,9H2,1
InchiKey: HMEWYCNQLMHIHU-HWKANZROSA-N
Formula: C13H14O3
SMILES: CCC(=O)C=CCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
gf	-0.75	kJ/mol	Joback Method
hf	-264.28	kJ/mol	Joback Method
hfus	37.51	kJ/mol	Joback Method
hvap	64.08	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.493		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1784.00		NIST Webbook
tb	656.82	K	Joback Method
tc	882.74	K	Joback Method
tf	407.90	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.84	J/mol×K	656.82	Joback Method
cpg	452.53	J/mol×K	694.47	Joback Method
cpg	465.27	J/mol×K	732.13	Joback Method
cpg	477.15	J/mol×K	769.78	Joback Method
cpg	488.24	J/mol×K	807.43	Joback Method
cpg	498.64	J/mol×K	845.09	Joback Method
cpg	508.44	J/mol×K	882.74	Joback Method
dvisc	0.0019334	Pa×s	407.90	Joback Method
dvisc	0.0012653	Pa×s	449.39	Joback Method

dvisc	0.0008895	Pa×s	490.87	Joback Method
dvisc	0.0006607	Pa×s	532.36	Joback Method
dvisc	0.0005123	Pa×s	573.85	Joback Method
dvisc	0.0004111	Pa×s	615.33	Joback Method
dvisc	0.0003392	Pa×s	656.82	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=R83952&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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