

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
rinpola	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0008895	Paxs	490.87	Joback Method
dvisc	0.0006607	Paxs	532.36	Joback Method
dvisc	0.0005123	Paxs	573.85	Joback Method
dvisc	0.0004111	Paxs	615.33	Joback Method
dvisc	0.0003392	Paxs	656.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R83952&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
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

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