2-Octanone, 8-(3,4-methylenedioxyphenyl)

Inchi: InChI=1S/C15H20O3/c1-12(16)6-4-2-3-5-7-13-8-9-14-15(10-13)18-11-17-14/h8-10H,2-7,
InchiKey: DBBLBCCPXKEKRW-UHFFFAOYSA-N
Formula: C15H20O3
SMILES: CC(=O)CCCCCCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 248.32

Physical Properties

Property code	Value	Unit	Source
gf	-64.13	kJ/mol	Joback Method
hf	-422.78	kJ/mol	Joback Method
hfus	42.49	kJ/mol	Joback Method
hvap	68.57	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.497		Crippen Method
mcvol	200.900	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	2017.00		NIST Webbook
rinpol	2017.00		NIST Webbook
tb	698.42	K	Joback Method
tc	908.87	K	Joback Method
tf	435.52	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.77	J/mol×K	698.42	Joback Method
cpg	580.01	J/mol×K	733.49	Joback Method
cpg	594.32	J/mol×K	768.57	Joback Method
cpg	607.75	J/mol×K	803.64	Joback Method
cpg	620.37	J/mol×K	838.72	Joback Method
cpg	632.24	J/mol×K	873.79	Joback Method
cpg	643.42	J/mol×K	908.87	Joback Method
dvisc	0.0019583	Pa×s	435.52	Joback Method

dvisc	0.0012641	Pa×s	479.34	Joback Method
dvisc	0.0008780	Pa×s	523.15	Joback Method
dvisc	0.0006452	Pa×s	566.97	Joback Method
dvisc	0.0004956	Pa×s	610.79	Joback Method
dvisc	0.0003943	Pa×s	654.60	Joback Method
dvisc	0.0003229	Pa×s	698.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R83948&Units=SI

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