3-Decanone, 1-(4-hydroxy-3-methoxyphenyl)-

Other names: Heptyl 4-hydroxy-3-methoxyphenethyl ketone
1-(4-Hydroxy-3-methoxyphenyl)decan-3-one
Paradol
[6]-Paradol
[6]-Gingerone
1-(4-hydroxy-3-methoxyphenyl)decan-5-one
Inchi: InChI=1S/C17H26O3/c1-3-4-5-6-7-8-15(18)11-9-14-10-12-16(19)17(13-14)20-2/h10,12-1
InchiKey: CZNLTCTYLMYLHL-UHFFFAOYSA-N
Formula: C17H26O3
SMILES: CCCCCCCC(=O)CCc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 278.39
CAS: 27113-22-0

Physical Properties

Property code	Value	Unit	Source
gf	-193.50	kJ/mol	Joback Method
hf	-591.26	kJ/mol	Joback Method
hfus	42.01	kJ/mol	Joback Method
hvap	78.54	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.263		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2232.00		NIST Webbook
rinpol	2218.00		NIST Webbook
rinpol	2218.00		NIST Webbook
rinpol	2232.00		NIST Webbook
ripol	3506.00		NIST Webbook
ripol	3506.00		NIST Webbook
tb	776.93	K	Joback Method
tc	980.70	K	Joback Method
tf	504.17	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.92	J/mol×K	776.93	Joback Method
cpg	785.84	J/mol×K	946.74	Joback Method
cpg	773.06	J/mol×K	912.78	Joback Method
cpg	759.64	J/mol×K	878.81	Joback Method
cpg	745.52	J/mol×K	844.85	Joback Method
cpg	730.63	J/mol×K	810.89	Joback Method
cpg	798.05	J/mol×K	980.70	Joback Method
dvisc	0.0000069	Pa×s	776.93	Joback Method
dvisc	0.0000102	Pa×s	731.47	Joback Method
dvisc	0.0000157	Pa×s	686.01	Joback Method
dvisc	0.0000257	Pa×s	640.55	Joback Method
dvisc	0.0000454	Pa×s	595.09	Joback Method
dvisc	0.0000882	Pa×s	549.63	Joback Method
dvisc	0.0001929	Pa×s	504.17	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=C27113220&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume