

Homofuraneol

Other names:	2-Ethyl-4-hydroxy-5-methyl-3(2H)-furanone 3(2H)-Furanone, 2-ethyl-4-hydroxy-5-methyl- 2-ethyl-4-hydroxy-5-methyl-3(2H)-furanone (homofuraneol) 4-hydroxy-2-ethyl-5methyl-3(2H)-furanone 4-Hydroxy-2-ethyl-5-methyl-3(2H)-furanone (HEMF) 4-hydroxy-2- or 5-ethyl-5- and 2-methyl-3(2H)-furanone 2(or 5)-ethyl-4-hydroxy-5(or 2)-methyl- 3(2H)-furanone (Homofuraneol) 2-ethyl-4-hydroxy-5-methyl-(2 H)-furanone (homofuraneol) ethyl 4-hydroxy-5-methyl-3(2H)-furanone (homofuraneol) 2-ethyl-4-hydroxy-5-methylfuran-3(2H)-one
Inchi:	InChI=1S/C7H10O3/c1-3-5-7(9)6(8)4(2)10-5/h5,8H,3H2,1-2H3
InchiKey:	GWCRPYGYVRXVLI-UHFFFAOYSA-N
Formula:	C7H10O3
SMILES:	CCC1OC(C)=C(O)C1=O
Mol. weight [g/mol]:	142.15

Physical Properties

Property code	Value	Unit	Source
gf	-290.22	kJ/mol	Joback Method
hf	-514.42	kJ/mol	Joback Method
hfus	19.84	kJ/mol	Joback Method
hvap	58.48	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.154		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
rinpol	1139.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1140.00		NIST Webbook

rinpol	1159.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1175.00	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1146.00	NIST Webbook
ripol	2059.00	NIST Webbook
ripol	2078.00	NIST Webbook
ripol	2105.00	NIST Webbook
ripol	2104.00	NIST Webbook
ripol	2088.00	NIST Webbook
ripol	2109.00	NIST Webbook
ripol	2079.00	NIST Webbook
ripol	2045.00	NIST Webbook
ripol	2070.00	NIST Webbook
ripol	2073.00	NIST Webbook
ripol	2083.00	NIST Webbook
ripol	2100.00	NIST Webbook
ripol	2086.00	NIST Webbook
ripol	2067.00	NIST Webbook
ripol	2105.00	NIST Webbook
ripol	2078.00	NIST Webbook
ripol	2097.00	NIST Webbook
ripol	2061.00	NIST Webbook
ripol	2050.00	NIST Webbook
ripol	2085.00	NIST Webbook
ripol	2107.00	NIST Webbook
ripol	2111.00	NIST Webbook
ripol	2095.00	NIST Webbook
ripol	2105.00	NIST Webbook
ripol	2101.00	NIST Webbook
ripol	2111.00	NIST Webbook
ripol	2107.00	NIST Webbook
ripol	2106.00	NIST Webbook
ripol	2070.00	NIST Webbook
ripol	2105.00	NIST Webbook
ripol	2105.00	NIST Webbook
ripol	2072.00	NIST Webbook
ripol	2095.00	NIST Webbook

ripol	2108.00		NIST Webbook
ripol	2112.00		NIST Webbook
ripol	2090.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2107.00		NIST Webbook
ripol	2083.00		NIST Webbook
ripol	2105.00		NIST Webbook
ripol	2059.00		NIST Webbook
ripol	2078.00		NIST Webbook
ripol	2085.00		NIST Webbook
ripol	2083.00		NIST Webbook
ripol	2111.00		NIST Webbook
tb	570.91	K	Joback Method
tc	774.52	K	Joback Method
tf	360.96	K	Joback Method
vc	0.402	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.78	J/mol×K	570.91	Joback Method
cpg	276.34	J/mol×K	604.85	Joback Method
cpg	286.45	J/mol×K	638.78	Joback Method
cpg	296.11	J/mol×K	672.72	Joback Method
cpg	305.30	J/mol×K	706.65	Joback Method
cpg	314.01	J/mol×K	740.59	Joback Method
cpg	322.24	J/mol×K	774.52	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C27538109&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
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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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