

trans-«beta»-Methyl-«gamma»-octalactone

Other names:	5-Butyl-4-methyldihydro-2(3H)-furanone, trans- trans-Whiskey lactone (E)-Whiskylactone t-Whiskylactone 2(3H)-Furanone, 5-butyldihydro-4-methyl-, trans- trans-4-Hydroxy-3-methyloctanoic acid, «gamma»-lactone
Inchi:	InChI=1S/C9H16O2/c1-3-4-5-8-7(2)6-9(10)11-8/h7-8H,3-6H2,1-2H3/t7-,8+/m0/s1
InchiKey:	WNVCMFHPRIBNCW-JGVFFNPUSA-N
Formula:	C9H16O2
SMILES:	CCCCC1OC(=O)CC1C
Mol. weight [g/mol]:	156.22

Physical Properties

Property code	Value	Unit	Source
gf	-154.97	kJ/mol	Joback Method
hf	-458.65	kJ/mol	Joback Method
h _{fus}	21.56	kJ/mol	Joback Method
h _{vap}	44.33	kJ/mol	Joback Method
log ₁₀ w _s	-2.22		Crippen Method
log _p	2.128		Crippen Method
m _{cvol}	134.250	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
ripol	1914.00		NIST Webbook
tb	510.70	K	Joback Method
tc	718.10	K	Joback Method
tf	292.64	K	Joback Method
vc	0.507	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
c _{pg}	323.83	J/mol×K	510.70	Joback Method
c _{pg}	340.60	J/mol×K	545.27	Joback Method
c _{pg}	356.64	J/mol×K	579.83	Joback Method

cpg	371.95	J/mol×K	614.40	Joback Method
cpg	386.53	J/mol×K	648.97	Joback Method
cpg	400.37	J/mol×K	683.53	Joback Method
cpg	413.48	J/mol×K	718.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39638670&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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