cis-«beta»-Methyl-«gamma»-octalactone

Other names:	cis-«beta»-Methyl-«gamma»-Octalactone cis-4-methyl-5-butyldihydro-2(3H)-furanone cis-5-Butyl-4-methyldihydrofuran-2(3H)-one (cis)-Oak-lactone (Z)-Oaklactone 5-Butyl-4-methyldihydro-2(3H)-furanone, (Z)- cis-Whiskey lactone 5-Butyldihydro-4-methyl-2(3H)-furanone (cis) (.+/-.)-cis-Whiskey lactone 5-Butyl-4-methyldihydro-2(3H)-furanone trans-«beta»-methyl-«gamma»-octalactone
Inchi:	InChI=1S/C9H16O2/c1-3-4-5-8-7(2)6-9(10)11-8/h7-8H,3-6H2,1-2H3/t7-,8-/m1/s1
InchiKey:	WNVCMFHPRIBNCW-HTQZYQBOSA-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
hfus	21.56	kJ/mol	Joback Method
hvap	44.33	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.128		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1340.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1343.80		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1333.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	1949.00		NIST Webbook

ripol	1953.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1953.00		NIST Webbook
tb	510.70	K	Joback Method
tc	718.10	K	Joback Method
tf	292.64	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.83	J/mol×K	510.70	Joback Method
cpg	340.60	J/mol×K	545.27	Joback Method
cpg	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

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=C55013326&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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

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