

Levogluconenone

Inchi:	InChI=1S/C6H6O3/c7-5-2-1-4-3-8-6(5)9-4/h1-2,4,6H,3H2
InchiKey:	HITOXZPZGPXYHY-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	O=C1C=CC2COC1O2
Mol. weight [g/mol]:	126.11
CAS:	37112-31-5

Physical Properties

Property code	Value	Unit	Source
gf	-167.93	kJ/mol	Joback Method
hf	-377.81	kJ/mol	Joback Method
hfus	20.06	kJ/mol	Joback Method
hvap	42.68	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	-0.133		Crippen Method
mcvol	82.690	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	479.58	K	Joback Method
tc	716.24	K	Joback Method
tf	308.34	K	Joback Method
vc	0.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.75	J/mol×K	479.58	Joback Method
cpg	202.19	J/mol×K	519.02	Joback Method
cpg	213.85	J/mol×K	558.47	Joback Method
cpg	224.74	J/mol×K	597.91	Joback Method
cpg	234.91	J/mol×K	637.35	Joback Method
cpg	244.37	J/mol×K	676.80	Joback Method
cpg	253.15	J/mol×K	716.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37112315&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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