LEVOGLUCOSENONE

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

Physical Properties

Property code	Value	Unit	Source
hfus	20.06	kJ/mol	Joback Method
logp	-0.133		Crippen Method
mcvol	82.690	ml/mol	McGowan 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

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume