6-Methyl-2-methylthio-4-pyrone

Other names: 2-Methyl-6-(methylthio)-4H-pyran-4-one
Inchi: InChI=1S/C7H8O2S/c1-5-3-6(8)4-7(9-5)10-2/h3-4H,1-2H3
InchiKey: RUFUDTITWMXMEV-UHFFFAOYSA-N
Formula: C7H8O2S
SMILES: CSc1cc(=O)cc(C)o1
Mol. weight [g/mol]: 156.20
CAS: 52911-99-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.85		Crippen Method
logp	1.670		Crippen Method
mcvol	113.820	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	87.40 ± 3.80	kJ/mol	410.50	NIST Webbook
hvapt	62.70	kJ/mol	409.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73265e+01
Coeff. B	-7.53895e+03
Temperature range (K), min.	442.46
Temperature range (K), max.	627.46

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52911996&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure