m-Dioxin, 6-methyl-

Inchi: InChI=1S/C5H8O2/c1-5-2-3-6-4-7-5/h2H,3-4H2,1H3
InchiKey: XZXHLKGJBTVUGT-UHFFFAOYSA-N
Formula: C5H8O2
SMILES: CC1=CCOCO1
Mol. weight [g/mol]: 100.12
CAS: 15973-03-2

Physical Properties

Property code	Value	Unit	Source
gf	-128.53	kJ/mol	Joback Method
hf	-289.56	kJ/mol	Joback Method
hfus	16.26	kJ/mol	Joback Method
hvap	37.44	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.895		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	4710.65	kPa	Joback Method
tb	396.06	K	Joback Method
tc	607.71	K	Joback Method
tf	224.15	K	Joback Method
vc	0.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.42	J/mol×K	396.06	Joback Method
cpg	191.35	J/mol×K	572.43	Joback Method
cpg	182.78	J/mol×K	537.16	Joback Method
cpg	173.72	J/mol×K	501.88	Joback Method
cpg	164.15	J/mol×K	466.61	Joback Method
cpg	154.05	J/mol×K	431.33	Joback Method
cpg	199.43	J/mol×K	607.71	Joback Method
dvisc	0.0003632	Pa×s	396.06	Joback Method
dvisc	0.0004842	Pa×s	367.41	Joback Method

dvisc	0.0006776	Pa×s	338.76	Joback Method
dvisc	0.0010090	Pa×s	310.10	Joback Method
dvisc	0.0016293	Pa×s	281.45	Joback Method
dvisc	0.0029331	Pa×s	252.80	Joback Method
dvisc	0.0061364	Pa×s	224.15	Joback Method

Sources

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=C15973032&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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