

1,4-Dioxane, 2,6-dimethyl-

Other names:	2,6-Dimethyl-1,4-dioxane p-Dioxane, 2,6-dimethyl-
Inchi:	InChI=1S/C6H12O2/c1-5-3-7-4-6(2)8-5/h5-6H,3-4H2,1-2H3
InchiKey:	JZUPYBRYQINNRE-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CC1COCC(C)O1
Mol. weight [g/mol]:	116.16
CAS:	10138-17-7

Physical Properties

Property code	Value	Unit	Source
gf	-155.86	kJ/mol	Joback Method
hf	-397.19	kJ/mol	Joback Method
hfus	20.16	kJ/mol	Joback Method
hvap	38.09	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.810		Crippen Method
mvol	96.280	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	672.00		NIST Webbook
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tb	405.46	K	Joback Method
tc	610.20	K	Joback Method
tf	213.66	K	Joback Method
vc	0.345	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.64	J/mol×K	405.46	Joback Method
cpg	259.54	J/mol×K	576.08	Joback Method
cpg	247.58	J/mol×K	541.95	Joback Method
cpg	235.02	J/mol×K	507.83	Joback Method
cpg	221.85	J/mol×K	473.71	Joback Method

cpg	208.06	J/mol×K	439.58	Joback Method
cpg	270.89	J/mol×K	610.20	Joback Method
dvisc	0.0003666	Paxs	405.46	Joback Method
dvisc	0.0004728	Paxs	373.49	Joback Method
dvisc	0.0006396	Paxs	341.53	Joback Method
dvisc	0.0009210	Paxs	309.56	Joback Method
dvisc	0.0014422	Paxs	277.59	Joback Method
dvisc	0.0025382	Paxs	245.63	Joback Method
dvisc	0.0052904	Paxs	213.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10138177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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