

1,3-Dioxane,2,4,6-trimethyl-,(2«alpha»,4«alpha»,6

Inchi:	InChI=1S/C7H14O2/c1-5-4-6(2)9-7(3)8-5/h5-7H,4H2,1-3H3/t5-,6-/m0/s1
InchiKey:	OQGOSNRNRKMTEX-WDSKDSINSA-N
Formula:	C7H14O2
SMILES:	CC1CC(C)OC(C)O1
Mol. weight [g/mol]:	130.18
CAS:	36402-73-0

Physical Properties

Property code	Value	Unit	Source
chl	-4265.50 ± 1.00	kJ/mol	NIST Webbook
gf	-155.15	kJ/mol	Joback Method
hf	-447.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-490.00 ± 2.00	kJ/mol	NIST Webbook
hfus	23.82	kJ/mol	Joback Method
hvap	43.00	kJ/mol	NIST Webbook
hvap	43.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-1.65		Crippen Method
logp	1.546		Crippen Method
mcvol	110.370	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
tb	423.67	K	Joback Method
tc	625.87	K	Joback Method
tf	220.69	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.41	J/molxK	423.67	Joback Method
cpg	307.54	J/molxK	592.17	Joback Method
cpg	294.21	J/molxK	558.47	Joback Method
cpg	280.24	J/molxK	524.77	Joback Method
cpg	265.62	J/molxK	491.07	Joback Method
cpg	250.34	J/molxK	457.37	Joback Method

cpg	320.21	J/mol×K	625.87	Joback Method
dvisc	0.0003500	Paxs	423.67	Joback Method
dvisc	0.0004342	Paxs	389.84	Joback Method
dvisc	0.0005612	Paxs	356.01	Joback Method
dvisc	0.0007653	Paxs	322.18	Joback Method
dvisc	0.0011227	Paxs	288.35	Joback Method
dvisc	0.0018235	Paxs	254.52	Joback Method
dvisc	0.0034365	Paxs	220.69	Joback Method

Sources

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=C36402730&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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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