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

Other names: m-Dioxane, 2,4,6-trimethyl-, cis-2,4,cis-2,6-
cis-2,4,6-Trimethyl-1,3-Dioxane
(2«alpha»,4«alpha»,6«alpha»)-2,4,6-Trimethyl-1,3-dioxane
cis-2-R-4-trans-6-Trimethyl-1,3-dioxane

Inchi: InChI=1S/C7H14O2/c1-5-4-6(2)9-7(3)8-5/h5-7H,4H2,1-3H3/t5-,6+,7-

InchiKey: OQGOSNRNRKMTEX-KVSKUHBBSA-N

Formula: C7H14O2

SMILES: CC1CC(C)OC(C)O1

Mol. weight [g/mol]: 130.18

CAS: 19145-91-6

Physical Properties

Property code	Value	Unit	Source
chl	-4267.10 ± 2.80	kJ/mol	NIST Webbook
gf	-155.15	kJ/mol	Joback Method
hf	-438.17	kJ/mol	Joback Method
hfl	-488.30 ± 2.80	kJ/mol	NIST Webbook
hfus	23.82	kJ/mol	Joback Method
hvap	40.01	kJ/mol	Joback Method
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/mol×K	423.67	Joback Method
cpg	250.34	J/mol×K	457.37	Joback Method
cpg	265.62	J/mol×K	491.07	Joback Method

cpg	280.24	J/mol×K	524.77	Joback Method
cpg	294.21	J/mol×K	558.47	Joback Method
cpg	307.54	J/mol×K	592.17	Joback Method
cpg	320.21	J/mol×K	625.87	Joback Method
dvisc	0.0034365	Pa×s	220.69	Joback Method
dvisc	0.0018235	Pa×s	254.52	Joback Method
dvisc	0.0011227	Pa×s	288.35	Joback Method
dvisc	0.0007653	Pa×s	322.18	Joback Method
dvisc	0.0005612	Pa×s	356.01	Joback Method
dvisc	0.0004342	Pa×s	389.84	Joback Method
dvisc	0.0003500	Pa×s	423.67	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C19145916&Units=SI

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