1,3-Dioxane, 4-(1-methylethyl)

Inchi: InChI=1S/C7H14O2/c1-6(2)7-3-4-8-5-9-7/h6-7H,3-5H2,1-2H3
InchiKey: KEAZEIMZENXSOH-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CC(C)C1CCOCO1
Mol. weight [g/mol]: 130.18

Physical Properties

Property code	Value	Unit	Source
gf	-142.17	kJ/mol	Joback Method
hf	-402.77	kJ/mol	Joback Method
hfus	18.16	kJ/mol	Joback Method
hvap	40.24	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.405		Crippen Method
mcvol	110.370	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	840.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	831.00		NIST Webbook
ripol	1060.00		NIST Webbook
ripol	1074.00		NIST Webbook
ripol	1060.00		NIST Webbook
tb	432.57	K	Joback Method
tc	640.51	K	Joback Method
tf	214.17	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.78	J/mol×K	432.57	Joback Method
cpg	249.64	J/mol×K	467.23	Joback Method
cpg	264.72	J/mol×K	501.88	Joback Method
cpg	279.04	J/mol×K	536.54	Joback Method

cpg	292.62	J/mol×K	571.20	Joback Method
cpg	305.46	J/mol×K	605.85	Joback Method
cpg	317.59	J/mol×K	640.51	Joback Method
dvisc	0.0145445	Pa×s	214.17	Joback Method
dvisc	0.0049623	Pa×s	250.57	Joback Method
dvisc	0.0022240	Pa×s	286.97	Joback Method
dvisc	0.0011942	Pa×s	323.37	Joback Method
dvisc	0.0007272	Pa×s	359.77	Joback Method
dvisc	0.0004851	Pa×s	396.17	Joback Method
dvisc	0.0003464	Pa×s	432.57	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=R409077&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume