3-Methyl-4,6-dioxanonane

Other names: Propoxy-(2-butoxy)methane
Inchi: InChI=1S/C8H18O2/c1-4-6-9-7-10-8(3)5-2/h8H,4-7H2,1-3H3
InchiKey: NPFCLWSPJBPJHY-UHFFFAOYSA-N
Formula: C8H18O2
SMILES: CCCOCOC(C)CC
Mol. weight [g/mol]: 146.23

Physical Properties

Property code	Value	Unit	Source
gf	-195.96	kJ/mol	Joback Method
hf	-478.17	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	37.83	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.186		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	899.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	885.00		NIST Webbook
tb	426.84	K	Joback Method
tc	594.62	K	Joback Method
tf	209.38	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.43	J/mol×K	426.84	Joback Method
cpg	342.91	J/mol×K	566.66	Joback Method
cpg	331.54	J/mol×K	538.70	Joback Method
cpg	319.80	J/mol×K	510.73	Joback Method
cpg	307.70	J/mol×K	482.77	Joback Method
cpg	295.24	J/mol×K	454.80	Joback Method

cpg	353.90	J/mol×K	594.62	Joback Method
dvisc	0.0001837	Pa×s	426.84	Joback Method
dvisc	0.0002462	Pa×s	390.60	Joback Method
dvisc	0.0003502	Pa×s	354.35	Joback Method
dvisc	0.0005397	Pa×s	318.11	Joback Method
dvisc	0.0009298	Pa×s	281.87	Joback Method
dvisc	0.0018809	Pa×s	245.62	Joback Method
dvisc	0.0048555	Pa×s	209.38	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U334823&Units=SI
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

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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