1,3-Dioxane, 4-(2-methylpropyl)

Inchi: InChI=1S/C8H16O2/c1-7(2)5-8-3-4-9-6-10-8/h7-8H,3-6H2,1-2H3
InchiKey: ZRTAVZIDNPIUIG-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CC(C)CC1CCOCO1
Mol. weight [g/mol]: 144.21

Physical Properties

Property code	Value	Unit	Source
gf	-133.75	kJ/mol	Joback Method
hf	-423.41	kJ/mol	Joback Method
hfus	20.75	kJ/mol	Joback Method
hvap	42.46	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.796		Crippen Method
mcvol	124.460	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
rinpol	938.00		NIST Webbook
rinpol	945.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1167.00		NIST Webbook
tb	455.45	K	Joback Method
tc	660.82	K	Joback Method
tf	225.44	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.54	J/mol×K	455.45	Joback Method
cpg	293.47	J/mol×K	489.68	Joback Method
cpg	309.55	J/mol×K	523.91	Joback Method
cpg	324.83	J/mol×K	558.14	Joback Method
cpg	339.30	J/mol×K	592.37	Joback Method

cpg	352.99	J/mol×K	626.60	Joback Method
cpg	365.92	J/mol×K	660.82	Joback Method
dvisc	0.0138481	Pa×s	225.44	Joback Method
dvisc	0.0046899	Pa×s	263.77	Joback Method
dvisc	0.0020906	Pa×s	302.11	Joback Method
dvisc	0.0011179	Pa×s	340.44	Joback Method
dvisc	0.0006785	Pa×s	378.78	Joback Method
dvisc	0.0004514	Pa×s	417.11	Joback Method
dvisc	0.0003217	Pa×s	455.45	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R409082&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

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

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