1,3-Dioxane, 2-methyl-4-(4-hydroxypentyl), 2S,4R

Inchi: InChI=1S/C10H20O3/c1-8(11)4-3-5-10-6-7-12-9(2)13-10/h8-11H,3-7H2,1-2H3/t8?,9-,10+

InchiKey: NSZRASDFTIVBDT-XVBQNVSMSA-N

Formula: C10H20O3

SMILES: CC(O)CCCC1CCOC(C)O1

Mol. weight [g/mol]: 188.26

Physical Properties

Property code	Value	Unit	Source
gf	-261.44	kJ/mol	Joback Method
hf	-637.26	kJ/mol	Joback Method
hfus	31.08	kJ/mol	Joback Method
hvap	63.28	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.689		Crippen Method
mcvol	158.510	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
ripol	2067.00		NIST Webbook
tb	588.72	K	Joback Method
tc	776.97	K	Joback Method
tf	304.56	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.54	J/mol×K	588.72	Joback Method
cpg	451.39	J/mol×K	620.10	Joback Method
cpg	466.46	J/mol×K	651.47	Joback Method
cpg	480.76	J/mol×K	682.85	Joback Method
cpg	494.30	J/mol×K	714.22	Joback Method
cpg	507.09	J/mol×K	745.60	Joback Method
cpg	519.16	J/mol×K	776.97	Joback Method
dvisc	0.0201762	Pa×s	304.56	Joback Method
dvisc	0.0046124	Pa×s	351.92	Joback Method

dvisc	0.0014965	Pa×s	399.28	Joback Method
dvisc	0.0006164	Pa×s	446.64	Joback Method
dvisc	0.0003010	Pa×s	494.00	Joback Method
dvisc	0.0001666	Pa×s	541.36	Joback Method
dvisc	0.0001014	Pa×s	588.72	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=R191954&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume