1,3-Dioxane, 2-(1-methylbutyl)-4-pentyl, 2S,4R

Inchi: InChI=1S/C14H28O2/c1-4-6-7-9-13-10-11-15-14(16-13)12(3)8-5-2/h12-14H,4-11H2,1-3H
InchiKey: SOAGWVHVXXGBSI-KFTPUPIBSA-N
Formula: C14H28O2
SMILES: CCCCCC1CCOC(C(C)CCC)O1
Mol. weight [g/mol]: 228.37

Physical Properties

Property code	Value	Unit	Source
gf	-90.94	kJ/mol	Joback Method
hf	-567.59	kJ/mol	Joback Method
hfus	37.36	kJ/mol	Joback Method
hvap	55.51	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.135		Crippen Method
mcvol	209.000	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
ripol	1575.00		NIST Webbook
ripol	1575.00		NIST Webbook
tb	588.06	K	Joback Method
tc	777.76	K	Joback Method
tf	288.82	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.70	J/mol×K	588.06	Joback Method
cpg	668.04	J/mol×K	746.14	Joback Method
cpg	650.95	J/mol×K	714.53	Joback Method
cpg	632.90	J/mol×K	682.91	Joback Method
cpg	613.85	J/mol×K	651.29	Joback Method
cpg	593.79	J/mol×K	619.68	Joback Method
cpg	684.19	J/mol×K	777.76	Joback Method
dvisc	0.0001956	Pa×s	588.06	Joback Method

dvisc	0.0002679	Pa×s	538.19	Joback Method
dvisc	0.0003914	Pa×s	488.31	Joback Method
dvisc	0.0006232	Pa×s	438.44	Joback Method
dvisc	0.0011182	Pa×s	388.57	Joback Method
dvisc	0.0023831	Pa×s	338.69	Joback Method
dvisc	0.0065960	Pa×s	288.82	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=R191716&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