1,3-Dioxane, 2,4-dipentyl, 2S,4R

Inchi: InChI=1S/C14H28O2/c1-3-5-7-9-13-11-12-15-14(16-13)10-8-6-4-2/h13-14H,3-12H2,1-2H
InchiKey: JTGGXBHDIVDFHP-UONOGXRCSA-N
Formula: C14H28O2
SMILES: CCCCCC1CCOC(CCCCC)O1
Mol. weight [g/mol]: 228.37

Physical Properties

Property code	Value	Unit	Source
gf	-88.50	kJ/mol	Joback Method
hf	-562.31	kJ/mol	Joback Method
hfus	40.88	kJ/mol	Joback Method
hvap	55.90	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.279		Crippen Method
mcvol	209.000	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
ripol	1765.00		NIST Webbook
ripol	1765.00		NIST Webbook
tb	588.50	K	Joback Method
tc	774.71	K	Joback Method
tf	303.82	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.41	J/mol×K	588.50	Joback Method
cpg	593.06	J/mol×K	619.54	Joback Method
cpg	612.73	J/mol×K	650.57	Joback Method
cpg	631.42	J/mol×K	681.61	Joback Method
cpg	649.17	J/mol×K	712.64	Joback Method
cpg	666.00	J/mol×K	743.68	Joback Method
cpg	681.92	J/mol×K	774.71	Joback Method
dvisc	0.0047334	Pa×s	303.82	Joback Method

dvisc	0.0019812	Pa×s	351.27	Joback Method
dvisc	0.0010203	Pa×s	398.71	Joback Method
dvisc	0.0006050	Pa×s	446.16	Joback Method
dvisc	0.0003967	Pa×s	493.61	Joback Method
dvisc	0.0002801	Pa×s	541.05	Joback Method
dvisc	0.0002092	Pa×s	588.50	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=R191761&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