1,3-Dioxane, 2-isopentyl-4-(2-pentenyl), 2S,4R

Inchi: InChI=1S/C14H26O2/c1-4-5-6-7-13-10-11-15-14(16-13)9-8-12(2)3/h5-6,12-14H,4,7-11H2
InchiKey: LZKQPIVTALJJKY-BUHQSOCUSA-N
Formula: C14H26O2
SMILES: CCC=CCC1CCOC(CCC(C)C)O1
Mol. weight [g/mol]: 226.35

Physical Properties

Property code	Value	Unit	Source
gf	-10.72	kJ/mol	Joback Method
hf	-450.37	kJ/mol	Joback Method
hfus	37.56	kJ/mol	Joback Method
hvap	55.47	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.910		Crippen Method
mcvol	204.700	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
ripol	1663.00		NIST Webbook
ripol	1663.00		NIST Webbook
tb	592.22	K	Joback Method
tc	789.59	K	Joback Method
tf	283.74	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.65	J/mol×K	592.22	Joback Method
cpg	574.47	J/mol×K	625.11	Joback Method
cpg	594.18	J/mol×K	658.01	Joback Method
cpg	612.82	J/mol×K	690.90	Joback Method
cpg	630.43	J/mol×K	723.80	Joback Method
cpg	647.04	J/mol×K	756.69	Joback Method
cpg	662.69	J/mol×K	789.59	Joback Method
dvisc	0.0062441	Pa×s	283.74	Joback Method

dvisc	0.0021488	Pa×s	335.15	Joback Method
dvisc	0.0009821	Pa×s	386.57	Joback Method
dvisc	0.0005394	Pa×s	437.98	Joback Method
dvisc	0.0003361	Pa×s	489.39	Joback Method
dvisc	0.0002291	Pa×s	540.81	Joback Method
dvisc	0.0001669	Pa×s	592.22	Joback Method

Sources

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=R191870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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