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

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

Physical Properties

Property code	Value	Unit	Source
gf	-8.28	kJ/mol	Joback Method
hf	-445.09	kJ/mol	Joback Method
hfus	41.08	kJ/mol	Joback Method
hvap	55.86	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.055		Crippen Method
mcvol	204.700	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
ripol	1834.00		NIST Webbook
ripol	1834.00		NIST Webbook
tb	592.66	K	Joback Method
tc	786.28	K	Joback Method
tf	298.74	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.34	J/mol×K	592.66	Joback Method
cpg	644.97	J/mol×K	754.01	Joback Method
cpg	628.62	J/mol×K	721.74	Joback Method
cpg	611.32	J/mol×K	689.47	Joback Method
cpg	593.02	J/mol×K	657.20	Joback Method
cpg	573.71	J/mol×K	624.93	Joback Method
cpg	660.40	J/mol×K	786.28	Joback Method
dvisc	0.0001786	Pa×s	592.66	Joback Method

dvisc	0.0002397	Pa×s	543.67	Joback Method
dvisc	0.0003409	Pa×s	494.69	Joback Method
dvisc	0.0005241	Pa×s	445.70	Joback Method
dvisc	0.0008959	Pa×s	396.71	Joback Method
dvisc	0.0017812	Pa×s	347.73	Joback Method
dvisc	0.0044366	Pa×s	298.74	Joback Method

Sources

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=R191974&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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