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

Inchi: InChI=1S/C12H22O2/c1-4-5-6-7-11-8-9-13-12(14-11)10(2)3/h5-6,10-12H,4,7-9H2,1-3H3
InchiKey: URODEFYSNWWYIU-CYLBZQBVSA-N
Formula: C12H22O2
SMILES: CCC=CCC1CCOC(C(C)C)O1
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-27.56	kJ/mol	Joback Method
hf	-409.09	kJ/mol	Joback Method
hfus	32.38	kJ/mol	Joback Method
hvap	51.02	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.130		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
ripol	1522.00		NIST Webbook
ripol	1522.00		NIST Webbook
tb	546.46	K	Joback Method
tc	749.53	K	Joback Method
tf	261.20	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.38	J/mol×K	546.46	Joback Method
cpg	469.38	J/mol×K	580.30	Joback Method
cpg	488.31	J/mol×K	614.15	Joback Method
cpg	506.20	J/mol×K	647.99	Joback Method
cpg	523.10	J/mol×K	681.84	Joback Method
cpg	539.02	J/mol×K	715.68	Joback Method
cpg	554.01	J/mol×K	749.53	Joback Method
dvisc	0.0072168	Pa×s	261.20	Joback Method

dvisc	0.0025199	Pa×s	308.74	Joback Method
dvisc	0.0011651	Pa×s	356.29	Joback Method
dvisc	0.0006460	Pa×s	403.83	Joback Method
dvisc	0.0004056	Pa×s	451.37	Joback Method
dvisc	0.0002783	Pa×s	498.92	Joback Method
dvisc	0.0002038	Pa×s	546.46	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=R191914&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