1,3-Dioxane, 2-isopropyl-4-pentyl, 2S,4R

Inchi: InChI=1S/C12H24O2/c1-4-5-6-7-11-8-9-13-12(14-11)10(2)3/h10-12H,4-9H2,1-3H3/t11-,1
InchiKey: CBGXGEQERKTMMU-NWDGAFQWSA-N
Formula: C12H24O2
SMILES: CCCCCC1CCOC(C(C)C)O1
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
gf	-107.78	kJ/mol	Joback Method
hf	-526.31	kJ/mol	Joback Method
hfus	32.18	kJ/mol	Joback Method
hvap	51.06	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.354		Crippen Method
mcvol	180.820	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
ripol	1471.00		NIST Webbook
tb	542.30	K	Joback Method
tc	736.78	K	Joback Method
tf	266.28	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.27	J/mol×K	542.30	Joback Method
cpg	487.52	J/mol×K	574.71	Joback Method
cpg	506.79	J/mol×K	607.13	Joback Method
cpg	525.09	J/mol×K	639.54	Joback Method
cpg	542.46	J/mol×K	671.96	Joback Method
cpg	558.91	J/mol×K	704.37	Joback Method
cpg	574.46	J/mol×K	736.78	Joback Method
dvisc	0.0076248	Pa×s	266.28	Joback Method
dvisc	0.0028036	Pa×s	312.28	Joback Method

dvisc	0.0013328	Pa×s	358.29	Joback Method
dvisc	0.0007505	Pa×s	404.29	Joback Method
dvisc	0.0004752	Pa×s	450.29	Joback Method
dvisc	0.0003275	Pa×s	496.30	Joback Method
dvisc	0.0002404	Pa×s	542.30	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=R191934&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