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

Inchi: InChI=1S/C12H24O2/c1-3-5-6-8-11-9-10-13-12(14-11)7-4-2/h11-12H,3-10H2,1-2H3/t11-
InchiKey: VAJGCFHWSCBHQP-NWDGAFQWSA-N
Formula: C12H24O2
SMILES: CCCCCC1CCOC(CCC)O1
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
gf	-105.34	kJ/mol	Joback Method
hf	-521.03	kJ/mol	Joback Method
hfus	35.70	kJ/mol	Joback Method
hvap	51.45	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.498		Crippen Method
mcvol	180.820	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
ripol	1568.00		NIST Webbook
ripol	1568.00		NIST Webbook
tb	542.74	K	Joback Method
tc	733.30	K	Joback Method
tf	281.28	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.04	J/mol×K	542.74	Joback Method
cpg	556.79	J/mol×K	701.54	Joback Method
cpg	540.63	J/mol×K	669.78	Joback Method
cpg	523.59	J/mol×K	638.02	Joback Method
cpg	505.66	J/mol×K	606.26	Joback Method
cpg	486.82	J/mol×K	574.50	Joback Method
cpg	572.09	J/mol×K	733.30	Joback Method
dvisc	0.0002557	Pa×s	542.74	Joback Method

dvisc	0.0003399	Pa×s	499.16	Joback Method
dvisc	0.0004772	Pa×s	455.59	Joback Method
dvisc	0.0007199	Pa×s	412.01	Joback Method
dvisc	0.0011968	Pa×s	368.43	Joback Method
dvisc	0.0022804	Pa×s	324.86	Joback Method
dvisc	0.0053056	Pa×s	281.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R192011&Units=SI
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

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