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

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

Physical Properties

Property code	Value	Unit	Source
gf	-25.12	kJ/mol	Joback Method
hf	-403.81	kJ/mol	Joback Method
hfus	35.90	kJ/mol	Joback Method
hvap	51.40	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.274		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
ripol	1631.00		NIST Webbook
tb	546.90	K	Joback Method
tc	745.76	K	Joback Method
tf	276.20	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.13	J/mol×K	546.90	Joback Method
cpg	468.65	J/mol×K	580.04	Joback Method
cpg	487.15	J/mol×K	613.19	Joback Method
cpg	504.67	J/mol×K	646.33	Joback Method
cpg	521.24	J/mol×K	679.48	Joback Method
cpg	536.89	J/mol×K	712.62	Joback Method
cpg	551.65	J/mol×K	745.76	Joback Method
dvisc	0.0049650	Pa×s	276.20	Joback Method
dvisc	0.0020428	Pa×s	321.32	Joback Method

dvisc	0.0010460	Pa×s	366.43	Joback Method
dvisc	0.0006202	Pa×s	411.55	Joback Method
dvisc	0.0004078	Pa×s	456.67	Joback Method
dvisc	0.0002891	Pa×s	501.78	Joback Method
dvisc	0.0002169	Pa×s	546.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R191994&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