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

Inchi: InChI=1S/C11H20O2/c1-3-5-6-7-10-8-9-12-11(4-2)13-10/h5-6,10-11H,3-4,7-9H2,1-2H3/b
InchiKey: YTXWLKKWFUDTMB-PFDYWKIBSA-N
Formula: C11H20O2
SMILES: CCC=CCC1CCOC(CC)O1
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
gf	-33.54	kJ/mol	Joback Method
hf	-383.17	kJ/mol	Joback Method
hfus	33.31	kJ/mol	Joback Method
hvap	49.18	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.884		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
ripol	1537.00		NIST Webbook
ripol	1537.00		NIST Webbook
tb	524.02	K	Joback Method
tc	725.72	K	Joback Method
tf	264.93	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.40	J/mol×K	524.02	Joback Method
cpg	418.35	J/mol×K	557.64	Joback Method
cpg	436.32	J/mol×K	591.25	Joback Method
cpg	453.32	J/mol×K	624.87	Joback Method
cpg	469.40	J/mol×K	658.49	Joback Method
cpg	484.58	J/mol×K	692.11	Joback Method
cpg	498.90	J/mol×K	725.72	Joback Method
dvisc	0.0051639	Pa×s	264.93	Joback Method

dvisc	0.0021541	Pa×s	308.11	Joback Method
dvisc	0.0011140	Pa×s	351.29	Joback Method
dvisc	0.0006656	Pa×s	394.48	Joback Method
dvisc	0.0004403	Pa×s	437.66	Joback Method
dvisc	0.0003136	Pa×s	480.84	Joback Method
dvisc	0.0002363	Pa×s	524.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R191830&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