

1,3-Dioxane, 2,2-dimethyl-4-(2-pentenyl), 4R

Inchi:	InChI=1S/C11H20O2/c1-4-5-6-7-10-8-9-12-11(2,3)13-10/h5-6,10H,4,7-9H2,1-3H3/b6-5+
InchiKey:	MCJLMZXXIYIDQK-PORFMDZSA-N
Formula:	C11H20O2
SMILES:	CCC=CCC1CCOC(C)(C)O1
Mol. weight [g/mol]:	184.28

Physical Properties

Property code	Value	Unit	Source
gf	-39.03	kJ/mol	Joback Method
hf	-367.93	kJ/mol	Joback Method
hfus	27.01	kJ/mol	Joback Method
hvap	48.03	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.884		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
tb	524.26	K	Joback Method
tc	734.24	K	Joback Method
tf	288.83	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.15	J/mol×K	524.26	Joback Method
cpg	418.05	J/mol×K	559.26	Joback Method
cpg	435.81	J/mol×K	594.25	Joback Method
cpg	452.53	J/mol×K	629.25	Joback Method
cpg	468.32	J/mol×K	664.24	Joback Method
cpg	483.30	J/mol×K	699.24	Joback Method
cpg	497.56	J/mol×K	734.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R191736&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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