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

Inchi: InChI=1S/C12H22O2/c1-4-6-7-8-11-9-10-13-12(3,5-2)14-11/h6-7,11H,4-5,8-10H2,1-3H3/
InchiKey: ZBHDHORAJVLHID-FNSAGKMKSA-N
Formula: C12H22O2
SMILES: CCC=CCC1CCOC(C)(CC)O1
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-30.61	kJ/mol	Joback Method
hf	-388.57	kJ/mol	Joback Method
hfus	29.60	kJ/mol	Joback Method
hvap	50.25	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.274		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
ripol	1550.00		NIST Webbook
ripol	1550.00		NIST Webbook
tb	547.14	K	Joback Method
tc	753.86	K	Joback Method
tf	300.10	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.38	J/mol×K	547.14	Joback Method
cpg	467.80	J/mol×K	581.59	Joback Method
cpg	486.09	J/mol×K	616.05	Joback Method
cpg	503.37	J/mol×K	650.50	Joback Method
cpg	519.74	J/mol×K	684.95	Joback Method
cpg	535.31	J/mol×K	719.41	Joback Method
cpg	550.19	J/mol×K	753.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R191796&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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