1,3-Dioxane, 2,2-dimethyl-4-pentyl, 4R

Inchi: InChI=1S/C11H22O2/c1-4-5-6-7-10-8-9-12-11(2,3)13-10/h10H,4-9H2,1-3H3/t10-/m0/s1
InchiKey: ADNZCWQGZVIHRC-JTQLQIEISA-N
Formula: C11H22O2
SMILES: CCCCCC1CCOC(C)(C)O1
Mol. weight [g/mol]: 186.29

Physical Properties

Property code	Value	Unit	Source
gf	-119.25	kJ/mol	Joback Method
hf	-485.15	kJ/mol	Joback Method
hfus	26.81	kJ/mol	Joback Method
hvap	48.07	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.108		Crippen Method
mcvol	166.730	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
ripol	1429.00		NIST Webbook
ripol	1429.00		NIST Webbook
tb	520.10	K	Joback Method
tc	720.79	K	Joback Method
tf	293.91	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.60	J/mol×K	520.10	Joback Method
cpg	435.80	J/mol×K	553.55	Joback Method
cpg	453.95	J/mol×K	587.00	Joback Method
cpg	471.13	J/mol×K	620.44	Joback Method
cpg	487.42	J/mol×K	653.89	Joback Method
cpg	502.92	J/mol×K	687.34	Joback Method
cpg	517.71	J/mol×K	720.79	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=R191756&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