

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

Inchi:	InChI=1S/C14H28O2/c1-3-5-7-9-13-11-12-15-14(16-13)10-8-6-4-2/h13-14H,3-12H2,1-2H
InchiKey:	JTGGXBHDIVDFHP-KBPBESRZSA-N
Formula:	C14H28O2
SMILES:	CCCCC1CCOC(CCCCC)O1
Mol. weight [g/mol]:	228.37

Physical Properties

Property code	Value	Unit	Source
gf	-88.50	kJ/mol	Joback Method
hf	-562.31	kJ/mol	Joback Method
hfus	40.88	kJ/mol	Joback Method
hvap	55.90	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.279		Crippen Method
mcvol	209.000	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
ripol	1847.00		NIST Webbook
ripol	1847.00		NIST Webbook
tb	588.50	K	Joback Method
tc	774.71	K	Joback Method
tf	303.82	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.41	J/molxK	588.50	Joback Method
cpg	666.00	J/molxK	743.68	Joback Method
cpg	649.17	J/molxK	712.64	Joback Method
cpg	631.42	J/molxK	681.61	Joback Method
cpg	612.73	J/molxK	650.57	Joback Method
cpg	593.06	J/molxK	619.54	Joback Method
cpg	681.92	J/molxK	774.71	Joback Method
dvisc	0.0002092	Paxs	588.50	Joback Method

dvisc	0.0002801	Paxs	541.05	Joback Method
dvisc	0.0003967	Paxs	493.61	Joback Method
dvisc	0.0006050	Paxs	446.16	Joback Method
dvisc	0.0010203	Paxs	398.71	Joback Method
dvisc	0.0019812	Paxs	351.27	Joback Method
dvisc	0.0047334	Paxs	303.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R191776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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