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

Inchi: InChI=1S/C11H22O2/c1-3-5-6-7-10-8-9-12-11(4-2)13-10/h10-11H,3-9H2,1-2H3/t10-,11-/
InchiKey: UCGYQTHBPZXKHC-QWRGUYRKSA-N
Formula: C11H22O2
SMILES: CCCCCC1CCOC(CC)O1
Mol. weight [g/mol]: 186.29

Physical Properties

Property code	Value	Unit	Source
gf	-113.76	kJ/mol	Joback Method
hf	-500.39	kJ/mol	Joback Method
hfus	33.11	kJ/mol	Joback Method
hvap	49.22	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.108		Crippen Method
mcvol	166.730	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
ripol	1560.00		NIST Webbook
ripol	1560.00		NIST Webbook
tb	519.86	K	Joback Method
tc	712.81	K	Joback Method
tf	270.01	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.76	J/mol×K	519.86	Joback Method
cpg	503.96	J/mol×K	680.65	Joback Method
cpg	488.24	J/mol×K	648.49	Joback Method
cpg	471.69	J/mol×K	616.34	Joback Method
cpg	454.26	J/mol×K	584.18	Joback Method
cpg	435.96	J/mol×K	552.02	Joback Method
cpg	518.84	J/mol×K	712.81	Joback Method
dvisc	0.0002794	Pa×s	519.86	Joback Method

dvisc	0.0003700	Pa×s	478.22	Joback Method
dvisc	0.0005170	Pa×s	436.58	Joback Method
dvisc	0.0007750	Pa×s	394.94	Joback Method
dvisc	0.0012782	Pa×s	353.29	Joback Method
dvisc	0.0024098	Pa×s	311.65	Joback Method
dvisc	0.0055245	Pa×s	270.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R191845&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

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