trans-2-Hexyl-5-methyl-1,3-dioxane

Inchi: InChI=1S/C11H22O2/c1-3-4-5-6-7-11-12-8-10(2)9-13-11/h10-11H,3-9H2,1-2H3/t10-,11-
InchiKey: ZOVQWQKIOCKGED-XYPYZODXSA-N
Formula: C11H22O2
SMILES: CCCCCCC1OCC(C)CO1
Mol. weight [g/mol]: 186.29
CAS: 41824-31-1

Physical Properties

Property code	Value	Unit	Source
chl	-6893.00 ± 13.00	kJ/mol	NIST Webbook
gf	-113.76	kJ/mol	Joback Method
hf	-500.39	kJ/mol	Joback Method
hfl	-580.00 ± 13.00	kJ/mol	NIST Webbook
hfus	33.11	kJ/mol	Joback Method
hvap	49.22	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.966		Crippen Method
mcvol	166.730	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
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	435.96	J/mol×K	552.02	Joback Method
cpg	454.26	J/mol×K	584.18	Joback Method
cpg	471.69	J/mol×K	616.34	Joback Method
cpg	488.24	J/mol×K	648.49	Joback Method
cpg	503.96	J/mol×K	680.65	Joback Method
cpg	518.84	J/mol×K	712.81	Joback Method

dvisc	0.0055245	Pa×s	270.01	Joback Method
dvisc	0.0024098	Pa×s	311.65	Joback Method
dvisc	0.0012782	Pa×s	353.29	Joback Method
dvisc	0.0007750	Pa×s	394.94	Joback Method
dvisc	0.0005170	Pa×s	436.58	Joback Method
dvisc	0.0003700	Pa×s	478.22	Joback Method
dvisc	0.0002794	Pa×s	519.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41824311&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.