2,4-Diisopropylhexahydropyrano[2,3-d] m-dioxin

Inchi: InChI=1S/C13H24O3/c1-8(2)11-10-6-5-7-14-13(10)16-12(15-11)9(3)4/h8-13H,5-7H2,1-4

InchiKey: UJXBOBIXMAERGY-UHFFFAOYSA-N

Formula: C13H24O3

SMILES: CC(C)C1OC2OCCCC2C(C(C)C)O1

Mol. weight [g/mol]: 228.33

CAS: 108989-86-2

Physical Properties

Property code	Value	Unit	Source
gf	-146.98	kJ/mol	Joback Method
hf	-637.93	kJ/mol	Joback Method
hfus	36.33	kJ/mol	Joback Method
hvap	57.18	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.793		Crippen Method
mcvol	189.920	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
tb	598.03	K	Joback Method
tc	813.07	K	Joback Method
tf	299.30	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.41	J/mol×K	598.03	Joback Method
cpg	568.15	J/mol×K	633.87	Joback Method
cpg	589.54	J/mol×K	669.71	Joback Method
cpg	609.61	J/mol×K	705.55	Joback Method
cpg	628.40	J/mol×K	741.39	Joback Method
cpg	645.94	J/mol×K	777.23	Joback Method
cpg	662.29	J/mol×K	813.07	Joback Method
dvisc	0.0059823	Pa×s	299.30	Joback Method
dvisc	0.0027681	Pa×s	349.09	Joback Method

dvisc	0.0015526	Pa×s	398.88	Joback Method
dvisc	0.0009901	Pa×s	448.66	Joback Method
dvisc	0.0006907	Pa×s	498.45	Joback Method
dvisc	0.0005144	Pa×s	548.24	Joback Method
dvisc	0.0004024	Pa×s	598.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108989862&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume