

d,L-1,2-Dimethyl-1,2-diphenylethylene glycol dimethyl ether

Inchi: InChI=1S/C18H22O2/c1-17(19-3,15-11-7-5-8-12-15)18(2,20-4)16-13-9-6-10-14-16/h5-14
InchiKey: MKOCHBGQRKMDTE-UHFFFAOYSA-N
Formula: C18H22O2
SMILES: COC(C)(c1ccccc1)C(C)(OC)c1ccccc1
Mol. weight [g/mol]: 270.37
CAS: 41047-48-7

Physical Properties

Property code	Value	Unit	Source
chs	-9929.90 ± 5.90	kJ/mol	NIST Webbook
gf	121.18	kJ/mol	Joback Method
hf	-183.00 ± 6.30	kJ/mol	NIST Webbook
hfus	18.01	kJ/mol	Joback Method
hvap	62.44	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	4.110		Crippen Method
mcvol	228.700	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
tb	702.98	K	Joback Method
tc	943.96	K	Joback Method
tf	394.76	K	Joback Method
vc	0.842	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.36	J/mol×K	903.80	Joback Method
cpg	734.97	J/mol×K	943.96	Joback Method
cpg	639.73	J/mol×K	702.98	Joback Method
cpg	659.23	J/mol×K	743.14	Joback Method
cpg	677.14	J/mol×K	783.31	Joback Method
cpg	693.55	J/mol×K	823.47	Joback Method
cpg	708.59	J/mol×K	863.63	Joback Method
dvisc	0.0000526	Paxs	702.98	Joback Method

dvisc	0.0000720	Paxs	651.61	Joback Method
dvisc	0.0011758	Paxs	394.76	Joback Method
dvisc	0.0005199	Paxs	446.13	Joback Method
dvisc	0.0002721	Paxs	497.50	Joback Method
dvisc	0.0001608	Paxs	548.87	Joback Method
dvisc	0.0001039	Paxs	600.24	Joback Method
hsubt	114.20 ± 6.30	kJ/mol	338.50	NIST Webbook
hsubt	114.00 ± 2.00	kJ/mol	303.00	NIST Webbook

Sources

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=C41047487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid 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
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

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