

ditolyl ether

Inchi:	InChI=1S/C14H14O/c1-11-5-3-7-13(9-11)15-14-8-4-6-12(2)10-14/h3-10H,1-2H3
InchiKey:	FDLFMPKQBNPIER-UHFFFAOYSA-N
Formula:	C14H14O
SMILES:	Cc1cccc(Oc2cccc(C)c2)c1
Mol. weight [g/mol]:	198.27

Physical Properties

Property code	Value	Unit	Source
gf	167.56	kJ/mol	Joback Method
hf	-14.39	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	55.04	kJ/mol	Joback Method
log10ws	-4.85		Aqueous Solubility Prediction Method
logp	4.096		Crippen Method
mcvol	166.470	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
tb	605.46	K	Joback Method
tc	843.53	K	Joback Method
tf	347.65	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.28	J/mol×K	605.46	Joback Method
cpg	413.91	J/mol×K	645.14	Joback Method
cpg	429.41	J/mol×K	684.82	Joback Method
cpg	443.82	J/mol×K	724.49	Joback Method
cpg	457.18	J/mol×K	764.17	Joback Method
cpg	469.52	J/mol×K	803.85	Joback Method
cpg	480.89	J/mol×K	843.53	Joback Method
dvisc	0.0011465	Pa×s	347.65	Joback Method
dvisc	0.0006664	Pa×s	390.62	Joback Method

dvisc	0.0004313	Pa×s	433.59	Joback Method
dvisc	0.0003019	Pa×s	476.56	Joback Method
dvisc	0.0002242	Pa×s	519.52	Joback Method
dvisc	0.0001742	Pa×s	562.49	Joback Method
dvisc	0.0001403	Pa×s	605.46	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

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