

Ethane, 1,1-di-o-tolyl-

Other names:	1,1-Di-o-tolylethane
Inchi:	InChI=1S/C16H18/c1-12-8-4-6-10-15(12)14(3)16-11-7-5-9-13(16)2/h4-11,14H,1-3H3
InchiKey:	QODLNWFFLYSPEP-UHFFFAOYSA-N
Formula:	C16H18
SMILES:	Cc1ccccc1C(C)c1ccccc1C
Mol. weight [g/mol]:	210.31
CAS:	33268-48-3

Physical Properties

Property code	Value	Unit	Source
chl	-8842.50 ± 2.00	kJ/mol	NIST Webbook
gf	286.96	kJ/mol	Joback Method
hf	71.27	kJ/mol	Joback Method
hfus	20.98	kJ/mol	Joback Method
hvap	56.70	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.455		Crippen Method
mcvol	188.780	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
tb	628.36	K	Joback Method
tc	865.27	K	Joback Method
tf	338.80 ± 0.80	K	NIST Webbook
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.16	J/mol×K	628.36	Joback Method
cpg	552.81	J/mol×K	825.78	Joback Method
cpg	539.02	J/mol×K	786.30	Joback Method
cpg	524.13	J/mol×K	746.81	Joback Method
cpg	508.06	J/mol×K	707.33	Joback Method
cpg	490.76	J/mol×K	667.84	Joback Method
cpg	565.57	J/mol×K	865.27	Joback Method

dvisc	0.0001369	Pa×s	628.36	Joback Method
dvisc	0.0001751	Pa×s	579.13	Joback Method
dvisc	0.0002344	Pa×s	529.89	Joback Method
dvisc	0.0003332	Pa×s	480.66	Joback Method
dvisc	0.0005132	Pa×s	431.43	Joback Method
dvisc	0.0008835	Pa×s	382.19	Joback Method
dvisc	0.0017859	Pa×s	332.96	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	https://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33268483&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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