

1,1-di-o-Tolyethylene

Inchi:	InChI=1S/C16H16/c1-12-8-4-6-10-15(12)14(3)16-11-7-5-9-13(16)2/h4-11H,3H2,1-2H3
InchiKey:	MUZMRKGPXHDTOF-UHFFFAOYSA-N
Formula:	C16H16
SMILES:	<chem>C=C(c1ccccc1C)c1ccccc1C</chem>
Mol. weight [g/mol]:	208.30
CAS:	2919-19-9

Physical Properties

Property code	Value	Unit	Source
chs	-8671.80 ± 2.00	kJ/mol	NIST Webbook
chs	-8531.00 ± 2.00	kJ/mol	NIST Webbook
gf	368.69	kJ/mol	Joback Method
hf	192.19	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	56.50	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.365		Crippen Method
mvol	184.480	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
tb	625.36	K	Joback Method
tc	866.59	K	Joback Method
tf	332.24	K	Joback Method
vc	0.698	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.64	J/mol×K	625.36	Joback Method
cpg	467.47	J/mol×K	665.56	Joback Method
cpg	484.01	J/mol×K	705.77	Joback Method
cpg	499.32	J/mol×K	745.97	Joback Method
cpg	513.50	J/mol×K	786.18	Joback Method
cpg	526.61	J/mol×K	826.38	Joback Method
cpg	538.73	J/mol×K	866.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.00 ± 2.00	K	0.10	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2919199&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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