

Tran 1,2-di-o-tolyethene

Inchi:	InChI=1S/C16H16/c1-13-7-3-5-9-15(13)11-12-16-10-6-4-8-14(16)2/h3-12H,1-2H3/b12-11
InchiKey:	ARZIVALJTPLLHF-VAWYXSNFSA-N
Formula:	C16H16
SMILES:	Cc1ccccc1C=Cc1ccccc1C
Mol. weight [g/mol]:	208.30
CAS:	36888-18-3

Physical Properties

Property code	Value	Unit	Source
chs	-8657.70 ± 2.00	kJ/mol	NIST Webbook
gf	369.62	kJ/mol	Joback Method
hf	193.77	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	57.04	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.474		Crippen Method
mcvol	184.480	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
tb	632.96	K	Joback Method
tc	875.04	K	Joback Method
tf	342.88	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.67	J/mol×K	632.96	Joback Method
cpg	526.73	J/mol×K	834.69	Joback Method
cpg	513.76	J/mol×K	794.34	Joback Method
cpg	499.75	J/mol×K	754.00	Joback Method
cpg	484.63	J/mol×K	713.65	Joback Method
cpg	468.30	J/mol×K	673.31	Joback Method
cpg	538.77	J/mol×K	875.04	Joback Method
dvisc	0.0001264	Pa×s	632.96	Joback Method

dvisc	0.0001590	Pa×s	584.61	Joback Method
dvisc	0.0002085	Pa×s	536.27	Joback Method
dvisc	0.0002885	Pa×s	487.92	Joback Method
dvisc	0.0004287	Pa×s	439.57	Joback Method
dvisc	0.0007027	Pa×s	391.23	Joback Method
dvisc	0.0013240	Pa×s	342.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36888183&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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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