1-(4-TOLYL)-1-CYCLOHEXENE

Other names: 1-(1-cyclohexen-1-yl)-4-methylbenzene
Inchi: InChI=1S/C13H16/c1-11-7-9-13(10-8-11)12-5-3-2-4-6-12/h5,7-10H,2-4,6H2,1H3
InchiKey: YAOVYZVTIFLTSH-UHFFFAOYSA-N
Formula: C13H16
SMILES: Cc1ccc(C2=CCCCC2)cc1
Mol. weight [g/mol]: 172.27

Physical Properties

Property code	Value	Unit	Source
hf	86.06	kJ/mol	Cheméo Relay (1.0)
hfus	14.67	kJ/mol	Joback Method
hvap	66.42	kJ/mol	Cheméo Relay (1.0)
ie	7.89	eV	Cheméo Relay (1.0)
log10ws	-4.39		Cheméo Relay (1.0)
logp	3.952		Crippen Method
mcvol	155.110	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
tb	550.17	K	Cheméo Relay (1.0)
tc	746.47	K	Cheméo Relay (1.0)
tf	271.67	K	Cheméo Relay (1.0)
vc	0.563	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.68	J/mol×K	556.86	Joback Method
cpg	459.92	J/mol×K	797.65	Joback Method
cpg	446.64	J/mol×K	757.52	Joback Method
cpg	432.27	J/mol×K	717.39	Joback Method
cpg	416.76	J/mol×K	677.25	Joback Method
cpg	400.03	J/mol×K	637.12	Joback Method
cpg	382.02	J/mol×K	596.99	Joback Method
dvisc	0.0004651	Pa×s	428.49	Joback Method
dvisc	0.0001822	Pa×s	556.86	Joback Method

dvisc	0.0002364	Pa×s	514.07	Joback Method
dvisc	0.0003215	Pa×s	471.28	Joback Method
dvisc	0.0026461	Pa×s	300.11	Joback Method
dvisc	0.0007301	Pa×s	385.69	Joback Method
dvisc	0.0012826	Pa×s	342.90	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1821234&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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