di-p-Tolylacetylene

Other names: 1-Methyl-4-[2-(4-methylphenyl)ethynyl]benzene
Inchi: InChI=1S/C16H14/c1-13-3-7-15(8-4-13)11-12-16-9-5-14(2)6-10-16/h3-10H,1-2H3
InchiKey: OFDOCXDLDQXWIX-UHFFFAOYSA-N
Formula: C16H14
SMILES: Cc1ccc(C#Cc2ccc(C)cc2)cc1
Mol. weight [g/mol]: 206.28
CAS: 2789-88-0

Physical Properties

Property code	Value	Unit	Source
gf	492.20	kJ/mol	Joback Method
hf	348.85	kJ/mol	Joback Method
hfus	27.62	kJ/mol	Joback Method
hvap	59.24	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.703		Crippen Method
mcvol	180.180	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
tb	637.80	K	Joback Method
tc	898.88	K	Joback Method
tf	408.00 ± 4.00	K	NIST Webbook
tf	408.00 ± 4.00	K	NIST Webbook
tf	410.40 ± 1.00	K	NIST Webbook
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.11	J/mol×K	637.80	Joback Method
cpg	447.72	J/mol×K	681.31	Joback Method
cpg	463.98	J/mol×K	724.83	Joback Method
cpg	478.96	J/mol×K	768.34	Joback Method
cpg	492.75	J/mol×K	811.85	Joback Method
cpg	505.42	J/mol×K	855.37	Joback Method

cpg	517.06	J/mol×K	898.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2789880&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

Legend

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume