3-Methylphenylacetylene

Other names: Benzene,1-ethynyl-3-methyl-
3-Methylethynylbenzene
1-Ethynyl-3-methylbenzene
Inchi: InChI=1S/C9H8/c1-3-9-6-4-5-8(2)7-9/h1,4-7H,2H3
InchiKey: RENYIDZOAFFNHC-UHFFFAOYSA-N
Formula: C9H8
SMILES: C#Cc1cccc(C)c1
Mol. weight [g/mol]: 116.16
CAS: 766-82-5

Physical Properties

Property code	Value	Unit	Source
affp	843.00	kJ/mol	NIST Webbook
basg	810.60	kJ/mol	NIST Webbook
gf	350.75	kJ/mol	Joback Method
hf	287.87	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	38.42	kJ/mol	Joback Method
ie	8.63 ± 0.02	eV	NIST Webbook
log10ws	-2.65		Crippen Method
logp	1.976		Crippen Method
mcvol	105.310	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	1011.00		NIST Webbook
ripol	1450.90		NIST Webbook
ripol	1450.90		NIST Webbook
tb	427.10	K	Joback Method
tc	652.10	K	Joback Method
tf	277.10	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	187.73	J/mol×K	427.10	Joback Method
cpg	199.55	J/mol×K	464.60	Joback Method
cpg	210.63	J/mol×K	502.10	Joback Method
cpg	221.00	J/mol×K	539.60	Joback Method
cpg	230.69	J/mol×K	577.10	Joback Method
cpg	239.74	J/mol×K	614.60	Joback Method
cpg	248.19	J/mol×K	652.10	Joback Method

Sources

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=C766825&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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