

2-(P-TOLYL)ETHYLAMINE

Other names:	Benzeneethanamine, 4-methyl- p-methylphenethylamine
Inchi:	InChI=1S/C9H13N/c1-8-2-4-9(5-3-8)6-7-10/h2-5H,6-7,10H2,1H3
InchiKey:	VKJXAQYPOTYDLO-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	Cc1ccc(CCN)cc1
Mol. weight [g/mol]:	135.21

Physical Properties

Property code	Value	Unit	Source
af	0.4914		Cheméo Relay (1.0)
gf	194.13	kJ/mol	Joback Method
hf	22.96	kJ/mol	Cheméo Relay (1.0)
hfus	17.92	kJ/mol	Joback Method
hvap	59.51	kJ/mol	Cheméo Relay (1.0)
ie	8.25	eV	Cheméo Relay (1.0)
log10ws	-1.68		Cheméo Relay (1.0)
logp	1.496		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
tb	487.20	K	NIST Webbook
tc	706.38	K	Cheméo Relay (1.0)
tf	326.89	K	Cheméo Relay (1.0)
vc	0.441	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.53	J/mol×K	509.51	Joback Method
cpg	285.22	J/mol×K	546.28	Joback Method
cpg	298.11	J/mol×K	583.04	Joback Method
cpg	310.23	J/mol×K	619.81	Joback Method
cpg	321.61	J/mol×K	656.58	Joback Method
cpg	332.28	J/mol×K	693.35	Joback Method

Sources

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=C3261629&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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