Benzene, 1-isocyano-2-methyl-

Other names: o-Tolyl isocyanide
2-Tolylisocyanide
Inchi: InChI=1S/C8H7N/c1-7-5-3-4-6-8(7)9-2/h3-6H,1H3
InchiKey: HGHZICGHCZFYNX-UHFFFAOYSA-N
Formula: C8H7N
SMILES: [C-]#[N+]c1ccccc1C
Mol. weight [g/mol]: 117.15
CAS: 10468-64-1

Physical Properties

Property code	Value	Unit	Source
gf	252.44	kJ/mol	Joback Method
hf	181.49	kJ/mol	Joback Method
hfus	11.63	kJ/mol	Joback Method
hvap	46.82	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	2.546		Crippen Method
mcvol	101.200	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
tb	516.18	K	Joback Method
tc	749.09	K	Joback Method
tf	283.85	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.15	J/mol×K	516.18	Joback Method
cpg	211.18	J/mol×K	555.00	Joback Method
cpg	220.58	J/mol×K	593.82	Joback Method
cpg	229.35	J/mol×K	632.64	Joback Method
cpg	237.53	J/mol×K	671.46	Joback Method
cpg	245.15	J/mol×K	710.28	Joback Method
cpg	252.23	J/mol×K	749.09	Joback Method

hvapt	48.50	kJ/mol	377.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10468641&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

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
hvapt:	Enthalpy of vaporization at a given temperature
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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