

Benzene, 1,1'-methylenebis[4-isocyano-

Other names:	Phenyl isocyanide, 4,4'-methylenebis-Benzene, 1,1'-methylenebis*4-isocyano-
Inchi:	InChI=1S/C15H10N2/c1-16-14-7-3-12(4-8-14)11-13-5-9-15(17-2)10-6-13/h3-10H,11H2
InchiKey:	SYRYWPVKZTYAFV-UHFFFAOYSA-N
Formula:	C15H10N2
SMILES:	[C-]#[N+]c1ccc(Cc2ccc([N+]#[C-])cc2)cc1
Mol. weight [g/mol]:	218.25
CAS:	956-62-7

Physical Properties

Property code	Value	Unit	Source
gf	547.34	kJ/mol	Joback Method
hf	426.95	kJ/mol	Joback Method
hfus	24.92	kJ/mol	Joback Method
hvap	75.82	kJ/mol	Joback Method
log10ws	-9.08		Crippen Method
logp	4.379		Crippen Method
mvol	177.450	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	810.08	K	Joback Method
tc	1068.09	K	Joback Method
tf	466.67	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.35	J/molxK	810.08	Joback Method
cpg	473.10	J/molxK	853.08	Joback Method
cpg	482.88	J/molxK	896.08	Joback Method
cpg	491.78	J/molxK	939.09	Joback Method
cpg	499.87	J/molxK	982.09	Joback Method
cpg	507.23	J/molxK	1025.09	Joback Method
cpg	513.92	J/molxK	1068.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=C956627&Units=SI

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
h vap:	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

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