

Benzenamine, N,N'-methanetetraylbis-

Other names:	Carbodiimide, diphenyl- Diphenylcarbodiimide N,N'-Diphenylcarbodiimide 1,3-Diphenylcarbodiimide N,N'-Methanetetraylbis(benzenamine) Carbodiimide Stabilizer 2013-P
Inchi:	InChI=1S/C13H10N2/c1-3-7-12(8-4-1)14-11-15-13-9-5-2-6-10-13/h1-10H
InchiKey:	CMESPBFDMPSIY-UHFFFAOYSA-N
Formula:	C13H10N2
SMILES:	C(=Nc1ccccc1)=Nc1ccccc1
Mol. weight [g/mol]:	194.23
CAS:	622-16-2

Physical Properties

Property code	Value	Unit	Source
chl	-6830.80 ± 3.70	kJ/mol	NIST Webbook
hf	371.41	kJ/mol	Joback Method
hfl	286.00 ± 3.70	kJ/mol	NIST Webbook
hvap	56.19	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.824		Crippen Method
mcvol	157.870	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
sl	330.00	J/mol×K	NIST Webbook
tb	702.67	K	Joback Method
tc	982.08	K	Joback Method
tt	287.41 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	304.60	J/mol×K	298.15	NIST Webbook
hfust	18.55	kJ/mol	287.41	NIST Webbook

hfust	18.55	kJ/mol	287.40	NIST Webbook
hfust	18.55	kJ/mol	287.40	NIST Webbook
hvapt	65.60	kJ/mol	549.50	NIST Webbook
sfust	64.54	J/mol×K	287.41	NIST Webbook

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=C622162&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tt:	Triple Point Temperature

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