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

Other names:

p,p'-Diphenylmethane diisocyanate
Isocyanic acid, methylenedi-p-phenylene ester
p,p'-Methylenebis[phenyl isocyanate]
Bis(p-isocyanatophenyl)methane
Bis(1,4-isocyanatophenyl)methane
Bis(4-isocyanatophenyl)methane
Caradate 30
Desmodur 44
Diphenylmethane diisocyanate
Diphenylmethane p,p'-diisocyanate
Diphenylmethane 4,4'-diisocyanate
Hylene M50
Isonate 125 MF
Isonate 125M
Methylenebis[p-phenyl isocyanate]
Methylenebis[p-phenylene isocyanate]
Methylenebis[4-isocyanatobenzene]
Methylenebis[4-phenyl isocyanate]
Methylenebis[4-phenylene isocyanate]
Methylenedi(p-phenyl isocyanate)
Methylenedi(p-phenylene diisocyanate)
Methylenedi(p-phenylene isocyanate)
MDI
MDR
Nacconate 300
4,4'-Diisocyanatodiphenylmethane
4,4'-Methylenebis[phenyl isocyanate]
4,4'-Methylenedi(phenylene isocyanate)
4,4'-Diphenylmethane diisocyanate
1,1'-Methylenebis(4-isocyanatobenzene)
NCI-C50668
Di-(4-isocyanatophenyl)methane
Difenil-metan-diisocianato
Diphenylmethan-4,4'-diisocyanat
Methylbisphenyl isocyanate
Methylene bisphenyl isocyanate
4,4'-Diisocyanate de diphenylmethane
4,4'-Methylenedi-p-phenylene diisocyanate
Difenylmethaan-dissocyanaat
Isonate

	4,4'-Methylenediphenyl isocyanate
	Rubinate 44
	UN 2489
	Diphenylmethane 4,4-diisocyanate
	Diphenylmethyl diisocyanate
	Methylene diphenyl diisocyanate
	Methylenedi-p-phenyl diisocyanate
	Nocconate 300
	Methylenebisphenylene diisocyanate
	4,4'-Methylenediphenyl diisocyanate
	Isocyanic acid, diphenylmethylene ester
	Diphenylmethylene diisocyanate
Inchi:	InChI=1S/C15H10N2O2/c18-10-16-14-5-1-12(2-6-14)9-13-3-7-15(8-4-13)17-11-19/h1-8H
InchiKey:	UPMLOUAZCHDJJD-UHFFFAOYSA-N
Formula:	C15H10N2O2
SMILES:	O=C=Nc1ccc(Cc2ccc(N=C=O)cc2)cc1
Mol. weight [g/mol]:	250.25
CAS:	101-68-8

Physical Properties

Property code	Value	Unit	Source
chl	-6912.00 ± 54.00	kJ/mol	NIST Webbook
chs	-7276.00 ± 13.00	kJ/mol	NIST Webbook
chs	-7279.00 ± 3.30	kJ/mol	NIST Webbook
hf	189.00 ± 21.00	kJ/mol	NIST Webbook
hfs	-56.00 ± 13.00	kJ/mol	NIST Webbook
hfs	-53.00 ± 3.30	kJ/mol	NIST Webbook
hvap	73.92	kJ/mol	Joback Method
log10ws	-12.54		Crippen Method
logp	3.212		Crippen Method
mcvol	189.190	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
ss	332.50	J/mol×K	NIST Webbook
ss	332.50	J/mol×K	NIST Webbook
tb	739.26	K	Joback Method
tc	984.01	K	Joback Method
tt	313.57 ± 0.02	K	NIST Webbook
tt	313.57 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	307.00	J/mol×K	298.15	NIST Webbook
cps	244.80	J/mol×K	334.00	NIST Webbook
cps	313.00	J/mol×K	300.00	NIST Webbook
hfust	27.30	kJ/mol	313.60	NIST Webbook
hfust	27.30	kJ/mol	313.57	NIST Webbook
hfust	27.30	kJ/mol	313.57	NIST Webbook
hsubt	27.30 ± 0.10	kJ/mol	313.60	NIST Webbook
hvapt	90.60	kJ/mol	486.00	NIST Webbook
hvapt	78.00 ± 2.00	kJ/mol	442.00	NIST Webbook
hvapt	93.80	kJ/mol	486.00	NIST Webbook
hvapt	90.50	kJ/mol	378.00	NIST Webbook
sfust	87.10	J/mol×K	313.57	NIST Webbook
sfust	87.10	J/mol×K	313.57	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C101688&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
chs: Standard solid enthalpy of combustion
cps: Solid phase heat capacity
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsubt: Enthalpy of sublimation 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tt:	Triple Point Temperature

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