

Benzene, 2,4-diisocyanato-1-methyl-

Other names:

2,4-Diisocyanato-1-methylbenzene
2,4-Diisocyanatotoluene
Isocyanic acid, 4-methyl-m-phenylene ester
4-Methyl-m-phenylene diisocyanate
4-Methyl-m-phenylene isocyanate
2,4-TDI
2,4-Toluene diisocyanate
2,4-Tolylene diisocyanate
Tolylene-2,4-diisocyanate
Toluylene-2,4-diisocyanate
4-Methyl-1,3-phenylene diisocyanate
Di-iso-cyanatoluene
Di-isocyanate de toluylene
Diisocyanat-toluol
NCI-C50533
Tolueen-diisocyanaat
Toluen-disocianato
Toluilenodwuzocyanian
Tuluylendiisocyanat
TDI
Cresorcinol diisocyanate
Desmodur T80
Hylene T
Hylene tcpa
Hylene tlc
Hylene tm
Hylene tm-65
Hylene trf
Mondur TD
Mondur TD-80
Mondur tds
Rcra waste number U223
Rubinate tdi 80/20
TDI-80
Tolyene 2,4-diisocyanate
Nacconate 100
NSC 4791
Toluene 2,4-diisocyanate

Inchi:

InChI=1S/C9H6N2O2/c1-7-2-3-8(10-5-12)4-9(7)11-6-13/h2-4H,1H3

InchiKey:

DVKJHBMWWAPEIU-UHFFFAOYSA-N

Formula: C₉H₆N₂O₂
SMILES: Cc1ccc(N=C=O)cc1N=C=O
Mol. weight [g/mol]: 174.16
CAS: 584-84-9

Physical Properties

Property code	Value	Unit	Source
chl	-4235.00	kJ/mol	NIST Webbook
hf	-26.32	kJ/mol	Joback Method
hvap	58.29	kJ/mol	Joback Method
log10ws	-10.91		Crippen Method
logp	1.930		Crippen Method
mcvol	128.410	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
tb	575.30	K	Joback Method
tc	802.50	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	287.80	J/mol×K	298.00	NIST Webbook
hvapt	59.70	kJ/mol	451.50	NIST Webbook
hvapt	59.50	kJ/mol	461.50	NIST Webbook
hvapt	61.30	kJ/mol	451.50	NIST Webbook
hvapt	57.70 ± 0.20	kJ/mol	403.00	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=C584849&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
hvac:	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

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