Tetramethylene diisocyanate

Other names:	Butane, 1,4-diisocyanato- 1,4-Diisocyanatobutane
Inchi:	InChI=1S/C6H8N2O2/c9-5-7-3-1-2-4-8-6-10/h1-4H2
InchiKey:	OVBFMUAFNIIQAL-UHFFFAOYSA-N
Formula:	C6H8N2O2
SMILES:	O=C=NCCCCN=C=O
Mol. weight [g/mol]:	140.14
CAS:	4538-37-8

Physical Properties

Property code	Value	Unit	Source
hf	-177.99	kJ/mol	Joback Method
hvap	48.01	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	0.438		Crippen Method
mcvol	109.900	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	470.02	K	Joback Method
tc	659.16	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.76	kJ/mol	184.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4538378&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

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	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