N,N-DIETHYL-O-TOLUIDINE

Other names:	2-(Dimethylamino)toluene
	N,N-Diethyl-2-methylaniline
	N,N-Diethyl-o-toluidinium ion
	o-Toluidine, N,N-diethyl-
Inchi:	InChI=1S/C11H17N/c1-4-12(5-2)11-9-7-6-8-10(11)3/h6-9H,4-5H2,1-3H3
InchiKey:	YQYUUNRAPYPAPC-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	CCN(CC)c1ccccc1C
Mol. weight [g/mol]:	163.26
CAS:	606-46-2

Physical Properties

Property code	Value	Unit	Source
af	0.4624		Cheméo Relay (1.0)
gf	255.30	kJ/mol	Joback Method
hf	3.59	kJ/mol	Cheméo Relay (1.0)
hfus	20.92	kJ/mol	Joback Method
hvap	59.12	kJ/mol	Cheméo Relay (1.0)
ie	7.09	eV	Cheméo Relay (1.0)
log10ws	-3.01		Cheméo Relay (1.0)
logp	2.841		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1193.00		NIST Webbook
ripol	1428.00		NIST Webbook
tb	497.94	K	Cheméo Relay (1.0)
tc	703.23	K	Cheméo Relay (1.0)
tf	238.87	K	Cheméo Relay (1.0)
vc	0.550	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.22	J/mol×K	495.18	Joback Method

cpg	350.65	J/mol×K	528.60	Joback Method
cpg	366.18	J/mol×K	562.02	Joback Method
cpg	380.85	J/mol×K	595.44	Joback Method
cpg	394.69	J/mol×K	628.86	Joback Method
cpg	407.74	J/mol×K	662.29	Joback Method
cpg	420.04	J/mol×K	695.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.31197e+01
Coeff. B	-3.66397e+03
Coeff. C	-7.51880e+01
Temperature range (K), min.	360.72
Temperature range (K), max.	544.44

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C606462&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume