

Urea, N-(4-chlorophenyl)-N,N'-dimethyl-

Other names:	Urea, N-(4-chlorophenyl)-N,N'-dimethyl-
Inchi:	InChI=1S/C9H11ClN2O/c1-11-9(13)12(2)8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)
InchiKey:	XZTUYISAOWDOSC-UHFFFAOYSA-N
Formula:	C9H11ClN2O
SMILES:	CNC(=O)N(C)c1ccc(Cl)cc1
Mol. weight [g/mol]:	198.65

Physical Properties

Property code	Value	Unit	Source
hfus	26.63	kJ/mol	Joback Method
ie	8.23	eV	Cheméo Relay (1.0)
log10ws	-2.36		Cheméo Relay (1.0)
logp	2.116		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
tb	566.25	K	Cheméo Relay (1.0)
tf	375.88	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.65	J/mol×K	590.89	Joback Method
cpg	350.07	J/mol×K	627.68	Joback Method
cpg	361.63	J/mol×K	664.48	Joback Method
cpg	372.36	J/mol×K	701.27	Joback Method
cpg	382.31	J/mol×K	738.07	Joback Method
cpg	391.52	J/mol×K	774.86	Joback Method
cpg	400.03	J/mol×K	811.66	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13578251&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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