

UREA, N,N'-BIS(3-METHYLPHENYL)-

Other names:	Carbanilide, 3,3'-dimethyl- Urea, 1,3-di(3-tolyl)- N,N'-(Di-m-methylphenyl)urea
Inchi:	InChI=1S/C15H16N2O/c1-11-5-3-7-13(9-11)16-15(18)17-14-8-4-6-12(2)10-14/h3-10H,1-
InchiKey:	UPUMJVLLEADOLKF-UHFFFAOYSA-N
Formula:	C15H16N2O
SMILES:	Cc1cccc(NC(=O)Nc2cccc(C)c2)c1
Mol. weight [g/mol]:	240.31

Physical Properties

Property code	Value	Unit	Source
af	0.7245		Cheméo Relay (1.0)
gf	330.84	kJ/mol	Joback Method
hf	-65.03	kJ/mol	Cheméo Relay (1.0)
hfus	33.71	kJ/mol	Joback Method
hvap	105.16	kJ/mol	Cheméo Relay (1.0)
ie	7.62	eV	Cheméo Relay (1.0)
log10ws	-4.75		Cheméo Relay (1.0)
logp	3.947		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
tb	618.21	K	Cheméo Relay (1.0)
tc	968.21	K	Cheméo Relay (1.0)
tf	435.42	K	Cheméo Relay (1.0)
vc	0.707	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.83	J/mol×K	760.13	Joback Method
cpg	557.06	J/mol×K	799.74	Joback Method
cpg	570.15	J/mol×K	839.35	Joback Method
cpg	582.16	J/mol×K	878.96	Joback Method
cpg	593.16	J/mol×K	918.57	Joback Method

cpg	603.20	J/mol×K	958.18	Joback Method
cpg	612.37	J/mol×K	997.79	Joback Method

Sources

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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620508&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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