

N-Methyl-N-phenyl N'-ethyl urea

Inchi:	InChI=1S/C10H14N2O/c1-3-11-10(13)12(2)9-7-5-4-6-8-9/h4-8H,3H2,1-2H3,(H,11,13)
InchiKey:	GOVFUKDUNFENCA-UHFFFAOYSA-N
Formula:	C10H14N2O
SMILES:	CCNC(=O)N(C)c1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	52073-04-8

Physical Properties

Property code	Value	Unit	Source
chs	-5631.20 ± 5.90	kJ/mol	NIST Webbook
gf	216.98	kJ/mol	Joback Method
hf	-4.78	kJ/mol	Joback Method
hfs	-304.70 ± 5.90	kJ/mol	NIST Webbook
hfus	25.42	kJ/mol	Joback Method
hvap	55.36	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.852		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
tb	571.36	K	Joback Method
tc	783.36	K	Joback Method
tf	310.20 ± 0.00	K	NIST Webbook
vc	0.546	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.17	J/mol×K	571.36	Joback Method
cpg	373.62	J/mol×K	606.69	Joback Method
cpg	387.12	J/mol×K	642.03	Joback Method
cpg	399.71	J/mol×K	677.36	Joback Method
cpg	411.44	J/mol×K	712.70	Joback Method
cpg	422.36	J/mol×K	748.03	Joback Method
cpg	432.51	J/mol×K	783.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52073048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
tf:	Normal melting (fusion) point
vc:	Critical Volume

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