

Urea, 1-methyl-3-(2-phenylethyl)-

Inchi:	InChI=1S/C10H14N2O/c1-11-10(13)12-8-7-9-5-3-2-4-6-9/h2-6H,7-8H2,1H3,(H2,11,12,13)
InchiKey:	YCLJQUVEVLDQHI-UHFFFAOYSA-N
Formula:	C10H14N2O
SMILES:	CNC(=O)NCCc1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	6953-30-6

Physical Properties

Property code	Value	Unit	Source
gf	195.59	kJ/mol	Joback Method
hf	-18.84	kJ/mol	Joback Method
hfus	27.49	kJ/mol	Joback Method
hvap	59.75	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.158		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
tb	609.09	K	Joback Method
tc	823.81	K	Joback Method
tf	384.13	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.64	J/mol×K	609.09	Joback Method
cpg	386.27	J/mol×K	644.88	Joback Method
cpg	399.01	J/mol×K	680.66	Joback Method
cpg	410.89	J/mol×K	716.45	Joback Method
cpg	421.95	J/mol×K	752.24	Joback Method
cpg	432.25	J/mol×K	788.03	Joback Method
cpg	441.81	J/mol×K	823.81	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6953306&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
hvac:	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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