

Urea), 1,1'-p-phenylenebis-(3-methyl-

Inchi:	InChI=1S/C10H14N4O2/c1-11-9(15)13-7-3-5-8(6-4-7)14-10(16)12-2/h3-6H,1-2H3,(H2,11
InchiKey:	YNKFUFKMBLAHJZ-UHFFFAOYSA-N
Formula:	C10H14N4O2
SMILES:	CNC(=O)Nc1ccc(NC(=O)NC)cc1
Mol. weight [g/mol]:	222.24
CAS:	94628-91-8

Physical Properties

Property code	Value	Unit	Source
gf	235.82	kJ/mol	Joback Method
hf	-35.95	kJ/mol	Joback Method
hfus	38.90	kJ/mol	Joback Method
hvap	80.03	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.189		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
tb	768.28	K	Joback Method
tc	988.47	K	Joback Method
tf	551.90	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.14	J/mol×K	768.28	Joback Method
cpg	494.19	J/mol×K	804.98	Joback Method
cpg	504.36	J/mol×K	841.68	Joback Method
cpg	513.71	J/mol×K	878.37	Joback Method
cpg	522.27	J/mol×K	915.07	Joback Method
cpg	530.08	J/mol×K	951.77	Joback Method
cpg	537.18	J/mol×K	988.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94628918&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
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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