

Urea, tetraphenyl-

Inchi:	InChI=1S/C25H20N2O/c28-25(26(21-13-5-1-6-14-21)22-15-7-2-8-16-22)27(23-17-9-3-10
InchiKey:	ZVWHURINXJWEER-UHFFFAOYSA-N
Formula:	C25H20N2O
SMILES:	O=C(N(c1ccccc1)c1ccccc1)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	364.44
CAS:	632-89-3

Physical Properties

Property code	Value	Unit	Source
gf	701.90	kJ/mol	Joback Method
hf	409.27	kJ/mol	Joback Method
hfus	44.31	kJ/mol	Joback Method
hvap	91.18	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.783		Crippen Method
mcvol	289.600	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
tb	956.87	K	Joback Method
tc	1225.35	K	Joback Method
tf	592.06	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.10	J/molxK	956.87	Joback Method
cpg	900.58	J/molxK	1001.62	Joback Method
cpg	913.85	J/molxK	1046.36	Joback Method
cpg	926.15	J/molxK	1091.11	Joback Method
cpg	937.72	J/molxK	1135.86	Joback Method
cpg	948.82	J/molxK	1180.60	Joback Method
cpg	959.67	J/molxK	1225.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C632893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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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