N,N-Ethylene bis(N',N,-diphenyl urea)

Inchi: InChI=1S/C28H26N4O2/c33-27(31(23-13-5-1-6-14-23)24-15-7-2-8-16-24)29-21-22-30-28
InchiKey: JMJOGHWYXVODDY-UHFFFAOYSA-N
Formula: C28H26N4O2
SMILES: O=C(NCCNC(=O)N(c1ccccc1)c1ccccc1)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 450.53
CAS: 6123-88-2

Physical Properties

Property code	Value	Unit	Source
chs	-14539.00 ± 15.00	kJ/mol	NIST Webbook
gf	777.02	kJ/mol	Joback Method
hf	341.71	kJ/mol	Joback Method
hfs	-195.00 ± 15.00	kJ/mol	NIST Webbook
hfus	63.88	kJ/mol	Joback Method
hvap	117.48	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.082		Crippen Method
mcvol	353.400	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
tb	1179.72	K	Joback Method
tc	1449.62	K	Joback Method
tf	781.12	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1175.66	J/mol×K	1179.72	Joback Method
cpg	1188.14	J/mol×K	1224.70	Joback Method
cpg	1200.36	J/mol×K	1269.69	Joback Method
cpg	1212.59	J/mol×K	1314.67	Joback Method
cpg	1225.10	J/mol×K	1359.65	Joback Method
cpg	1238.16	J/mol×K	1404.64	Joback Method
cpg	1252.05	J/mol×K	1449.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6123882&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

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