4,4'-Methylene di-carbanilide

Inchi: InChI=1S/C27H24N4O2/c32-26(28-22-7-3-1-4-8-22)30-24-15-11-20(12-16-24)19-21-13-1
InchiKey: AFGPVXVFZRRJGM-UHFFFAOYSA-N
Formula: C27H24N4O2
SMILES: O=C(Nc1ccccc1)Nc1ccc(Cc2ccc(NC(=O)Nc3ccccc3)cc2)cc1
Mol. weight [g/mol]: 436.51
CAS: 13140-83-5

Physical Properties

Property code	Value	Unit	Source
gf	706.56	kJ/mol	Joback Method
hf	311.29	kJ/mol	Joback Method
hfus	64.67	kJ/mol	Joback Method
hvap	125.36	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.565		Crippen Method
mcvol	339.310	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
tb	1242.26	K	Joback Method
tc	1523.32	K	Joback Method
tf	835.27	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.02	J/mol×K	1242.26	Joback Method
cpg	1133.74	J/mol×K	1289.10	Joback Method
cpg	1143.03	J/mol×K	1335.95	Joback Method
cpg	1152.12	J/mol×K	1382.79	Joback Method
cpg	1161.25	J/mol×K	1429.63	Joback Method
cpg	1170.67	J/mol×K	1476.48	Joback Method
cpg	1180.60	J/mol×K	1523.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13140835&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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