Triazole, 3h-1,2,4-,5-amino-3-anilino-

Inchi: InChI=1S/C8H9N5/c9-7-11-8(13-12-7)10-6-4-2-1-3-5-6/h1-5,8,10H,(H2,9,11)
InchiKey: HPJAVIXGHSANOQ-UHFFFAOYSA-N
Formula: C8H9N5
SMILES: NC1=NC(Nc2ccccc2)N=N1
Mol. weight [g/mol]: 175.19

Physical Properties

Property code	Value	Unit	Source
gf	721.91	kJ/mol	Joback Method
hf	492.82	kJ/mol	Joback Method
hfus	32.22	kJ/mol	Joback Method
hvap	72.89	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.163		Crippen Method
mcvol	130.260	ml/mol	McGowan Method
pc	5527.84	kPa	Joback Method
tb	711.50	K	Joback Method
tc	997.19	K	Joback Method
tf	581.82	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.35	J/mol×K	711.50	Joback Method
cpg	417.11	J/mol×K	759.11	Joback Method
cpg	431.01	J/mol×K	806.73	Joback Method
cpg	443.04	J/mol×K	854.34	Joback Method
cpg	453.17	J/mol×K	901.96	Joback Method
cpg	461.38	J/mol×K	949.57	Joback Method
cpg	467.66	J/mol×K	997.19	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007333&Units=SI

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