

3-Phenyl-p-anisidine

Inchi:	InChI=1S/C13H13NO/c1-15-13-8-7-11(14)9-12(13)10-5-3-2-4-6-10/h2-9H,14H2,1H3
InchiKey:	OFBRKDXLBOTZNB-UHFFFAOYSA-N
Formula:	C13H13NO
SMILES:	COc1ccc(N)cc1-c1ccccc1
Mol. weight [g/mol]:	199.25
CAS:	56970-26-4

Physical Properties

Property code	Value	Unit	Source
gf	225.59	kJ/mol	Joback Method
hf	40.04	kJ/mol	Joback Method
hfus	23.12	kJ/mol	Joback Method
hvap	63.46	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.944		Crippen Method
mcvol	162.360	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
tb	655.11	K	Joback Method
tc	904.74	K	Joback Method
tf	419.64	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.08	J/molxK	655.11	Joback Method
cpg	423.20	J/molxK	696.72	Joback Method
cpg	437.17	J/molxK	738.32	Joback Method
cpg	450.03	J/molxK	779.93	Joback Method
cpg	461.82	J/molxK	821.53	Joback Method
cpg	472.59	J/molxK	863.14	Joback Method
cpg	482.38	J/molxK	904.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56970264&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

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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