

N-iso amyl aniline

Inchi:	InChI=1S/C11H17N/c1-3-10(2)9-12-11-7-5-4-6-8-11/h4-8,10,12H,3,9H2,1-2H3
InchiKey:	JIWKXBBRZYONNG-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	CCC(C)CNc1ccccc1
Mol. weight [g/mol]:	163.26

Physical Properties

Property code	Value	Unit	Source
gf	241.10	kJ/mol	Joback Method
hf	14.35	kJ/mol	Joback Method
hfus	19.86	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	3.145		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
tb	527.49	K	Joback Method
tc	735.29	K	Joback Method
tf	277.81	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.84	J/molxK	527.49	Joback Method
cpg	367.24	J/molxK	562.12	Joback Method
cpg	382.70	J/molxK	596.76	Joback Method
cpg	397.25	J/molxK	631.39	Joback Method
cpg	410.92	J/molxK	666.02	Joback Method
cpg	423.77	J/molxK	700.66	Joback Method
cpg	435.81	J/molxK	735.29	Joback Method

Sources

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=B6000177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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