N-amyl aniline

Other names: N-pentylaniline
Inchi: InChI=1S/C11H17N/c1-2-3-7-10-12-11-8-5-4-6-9-11/h4-6,8-9,12H,2-3,7,10H2,1H3
InchiKey: UMNSMBWAESLVOC-UHFFFAOYSA-N
Formula: C11H17N
SMILES: CCCCCNc1ccccc1
Mol. weight [g/mol]: 163.26
CAS: 2655-27-8

Physical Properties

Property code	Value	Unit	Source
gf	243.54	kJ/mol	Joback Method
hf	19.63	kJ/mol	Joback Method
hfus	23.39	kJ/mol	Joback Method
hvap	48.79	kJ/mol	Joback Method
ie	7.50	eV	NIST Webbook
log10ws	-3.15		Crippen Method
logp	3.289		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
tb	531.15 ± 6.00	K	NIST Webbook
tc	731.26	K	Joback Method
tf	292.81	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.57	J/mol×K	527.93	Joback Method
cpg	366.56	J/mol×K	561.82	Joback Method
cpg	381.64	J/mol×K	595.71	Joback Method
cpg	395.87	J/mol×K	629.60	Joback Method
cpg	409.26	J/mol×K	663.49	Joback Method
cpg	421.86	J/mol×K	697.37	Joback Method
cpg	433.71	J/mol×K	731.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48853e+01
Coeff. B	-4.54150e+03
Coeff. C	-8.88100e+01
Temperature range (K), min.	399.92
Temperature range (K), max.	563.18

Sources

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=C2655278&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume