

Aniline, n-ethyl-p-pentyl

Inchi:	InChI=1S/C13H21N/c1-3-5-6-7-12-8-10-13(11-9-12)14-4-2/h8-11,14H,3-7H2,1-2H3
InchiKey:	LLCICSCPINCSQS-UHFFFAOYSA-N
Formula:	C13H21N
SMILES:	CCCCCc1ccc(NCC)cc1
Mol. weight [g/mol]:	191.31
CAS:	116296-05-0

Physical Properties

Property code	Value	Unit	Source
gf	250.75	kJ/mol	Joback Method
hf	-33.12	kJ/mol	Joback Method
hfus	28.18	kJ/mol	Joback Method
hvap	53.91	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.851		Crippen Method
mcvol	180.250	ml/mol	McGowan Method
pc	2189.73	kPa	Joback Method
tb	578.67	K	Joback Method
tc	777.26	K	Joback Method
tf	327.87	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.98	J/molxK	578.67	Joback Method
cpg	464.94	J/molxK	611.77	Joback Method
cpg	480.99	J/molxK	644.87	Joback Method
cpg	496.17	J/molxK	677.97	Joback Method
cpg	510.52	J/molxK	711.06	Joback Method
cpg	524.06	J/molxK	744.16	Joback Method
cpg	536.83	J/molxK	777.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116296050&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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