

Aniline, n-hexadecyl-

Inchi:	InChI=1S/C22H39N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-21-23-22-19-16-15-17-20-22/
InchiKey:	IXEGRINNWXKNJO-UHFFFAOYSA-N
Formula:	C22H39N
SMILES:	CCCCCCCCCCCCCCCCNc1ccccc1
Mol. weight [g/mol]:	317.55
CAS:	4439-42-3

Physical Properties

Property code	Value	Unit	Source
gf	336.16	kJ/mol	Joback Method
hf	-207.41	kJ/mol	Joback Method
hfus	51.88	kJ/mol	Joback Method
hvap	73.28	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	7.580		Crippen Method
mcvol	307.060	ml/mol	McGowan Method
pc	1121.55	kPa	Joback Method
tb	779.61	K	Joback Method
tc	966.32	K	Joback Method
tf	416.78	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.39	J/molxK	779.61	Joback Method
cpg	972.39	J/molxK	810.73	Joback Method
cpg	991.30	J/molxK	841.85	Joback Method
cpg	1009.19	J/molxK	872.96	Joback Method
cpg	1026.11	J/molxK	904.08	Joback Method
cpg	1042.11	J/molxK	935.20	Joback Method
cpg	1057.24	J/molxK	966.32	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=C4439423&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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