Hexanenitrile, 6-amino-

Other names:	«omega»-Aminocapronitrile
	6-Aminocapronitrile
	6-Aminohexanenitrile
	6-aminohexanonitrile
Inchi:	InChI=1S/C6H12N2/c7-5-3-1-2-4-6-8/h1-5,7H2
InchiKey:	KBMSFJFLSXLIDJ-UHFFFAOYSA-N
Formula:	C6H12N2
SMILES:	N#CCCCCCN
Mol. weight [g/mol]:	112.17
CAS:	2432-74-8

Physical Properties

Property code	Value	Unit	Source
gf	199.27	kJ/mol	Joback Method
hf	31.50	kJ/mol	Joback Method
hfus	18.00	kJ/mol	Joback Method
hvap	50.07	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.029		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
tb	511.29	K	Joback Method
tc	711.96	K	Joback Method
tf	305.63	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.94	J/mol×K	511.29	Joback Method
cpg	248.71	J/mol×K	544.73	Joback Method
cpg	258.02	J/mol×K	578.18	Joback Method
cpg	266.87	J/mol×K	611.62	Joback Method
cpg	275.28	J/mol×K	645.07	Joback Method

cpg	283.27	J/mol×K	678.51	Joback Method
cpg	290.85	J/mol×K	711.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	401.20	K	3.60	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2432748&Units=SI

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume