6-Aminoundecane

Other names: 1-Pentylhexylamine
6-Aminoundecane
6-Undecanamine
Inchi: InChI=1S/C11H25N/c1-3-5-7-9-11(12)10-8-6-4-2/h11H,3-10,12H2,1-2H3
InchiKey: GFBRYGJZWXLRFR-UHFFFAOYSA-N
Formula: C11H25N
SMILES: CCCCCC(N)CCCCC
Mol. weight [g/mol]: 171.33

Physical Properties

Property code	Value	Unit	Source
af	0.5905		Cheméo Relay (1.0)
gf	105.75	kJ/mol	Joback Method
hf	-245.49	kJ/mol	Cheméo Relay (1.0)
hfus	25.92	kJ/mol	Joback Method
hvap	61.00	kJ/mol	Cheméo Relay (1.0)
ie	8.47	eV	Cheméo Relay (1.0)
log10ws	-4.45		Cheméo Relay (1.0)
logp	3.474		Crippen Method
mcvol	175.830	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
tb	489.08	K	Cheméo Relay (1.0)
tc	662.84	K	Cheméo Relay (1.0)
tf	261.00	K	Cheméo Relay (1.0)
vc	0.657	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.51	J/mol×K	523.17	Joback Method
cpg	447.00	J/mol×K	552.55	Joback Method
cpg	462.80	J/mol×K	581.94	Joback Method
cpg	477.92	J/mol×K	611.32	Joback Method
cpg	492.37	J/mol×K	640.70	Joback Method

cpg	506.19	J/mol×K	670.09	Joback Method
cpg	519.38	J/mol×K	699.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33788000&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume