3-Aminoheptane

Other names: 1-ethylpentylamine
3-Heptanamine
3-Heptylamine
Inchi: InChI=1S/C7H17N/c1-3-5-6-7(8)4-2/h7H,3-6,8H2,1-2H3
InchiKey: SRMHHEPXZLWKOK-UHFFFAOYSA-N
Formula: C7H17N
SMILES: CCCCC(N)CC
Mol. weight [g/mol]: 115.22
CAS: 28292-42-4

Physical Properties

Property code	Value	Unit	Source
gf	72.07	kJ/mol	Joback Method
hf	-159.30	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	41.43	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.914		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	868.00		NIST Webbook
ripol	1137.00		NIST Webbook
tb	414.15 ± 3.00	K	NIST Webbook
tc	614.39	K	Joback Method
tf	236.91	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.75	J/mol×K	431.65	Joback Method
cpg	263.71	J/mol×K	462.11	Joback Method
cpg	276.13	J/mol×K	492.56	Joback Method
cpg	288.03	J/mol×K	523.02	Joback Method

cpg	299.42	J/mol×K	553.48	Joback Method
cpg	310.31	J/mol×K	583.94	Joback Method
cpg	320.73	J/mol×K	614.39	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56583e+01
Coeff. B	-3.95082e+03
Coeff. C	-5.62840e+01
Temperature range (K), min.	313.32
Temperature range (K), max.	438.12

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=C28292424&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume