p-Heptylaniline

Other names: 4-Heptylaniline
Inchi: InChI=1S/C13H21N/c1-2-3-4-5-6-7-12-8-10-13(14)11-9-12/h8-11H,2-7,14H2,1H3
InchiKey: BNEWZYZRLNNWNR-UHFFFAOYSA-N
Formula: C13H21N
SMILES: CCCCCCCc1ccc(N)cc1
Mol. weight [g/mol]: 191.31
CAS: 37529-27-4

Physical Properties

Property code	Value	Unit	Source
gf	227.81	kJ/mol	Joback Method
hf	-52.80	kJ/mol	Joback Method
hfus	28.28	kJ/mol	Joback Method
hvap	58.11	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.782		Crippen Method
mcvol	180.250	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
tb	601.03	K	Joback Method
tc	807.53	K	Joback Method
tf	358.47	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.62	J/mol×K	601.03	Joback Method
cpg	477.34	J/mol×K	635.45	Joback Method
cpg	493.13	J/mol×K	669.86	Joback Method
cpg	508.01	J/mol×K	704.28	Joback Method
cpg	522.04	J/mol×K	738.70	Joback Method
cpg	535.24	J/mol×K	773.11	Joback Method
cpg	547.66	J/mol×K	807.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.50 ± 0.50	K	0.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50187e+01
Coeff. B	-4.72795e+03
Coeff. C	-9.40500e+01
Temperature range (K), min.	415.00
Temperature range (K), max.	581.10

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37529274&Units=SI

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

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

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