N-sec-Butylaniline

Inchi: InChI=1S/C10H15N/c1-3-9(2)11-10-7-5-4-6-8-10/h4-9,11H,3H2,1-2H3
InchiKey: LAMTXWQPHWUMLX-UHFFFAOYSA-N
Formula: C10H15N
SMILES: CCC(C)Nc1ccccc1
Mol. weight [g/mol]: 149.23
CAS: 6068-69-5

Physical Properties

Property code	Value	Unit	Source
gf	232.68	kJ/mol	Joback Method
hf	34.99	kJ/mol	Joback Method
hfus	17.27	kJ/mol	Joback Method
hvap	46.18	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.897		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	1223.20		NIST Webbook
tb	504.61	K	Joback Method
tc	715.64	K	Joback Method
tf	266.54	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.75	J/mol×K	504.61	Joback Method
cpg	320.38	J/mol×K	539.78	Joback Method
cpg	335.09	J/mol×K	574.95	Joback Method
cpg	348.92	J/mol×K	610.13	Joback Method
cpg	361.90	J/mol×K	645.30	Joback Method
cpg	374.08	J/mol×K	680.47	Joback Method
cpg	385.49	J/mol×K	715.64	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36839e+01
Coeff. B	-3.93695e+03
Coeff. C	-7.96360e+01
Temperature range (K), min.	373.52
Temperature range (K), max.	549.87

Sources

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=C6068695&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

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
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume