o-aminobutylbenzene

Other names: Benzenamine, 2-butyl-
o-butyl-aniline
Inchi: InChI=1S/C10H15N/c1-2-3-6-9-7-4-5-8-10(9)11/h4-5,7-8H,2-3,6,11H2,1H3
InchiKey: HDVUPIFFKAHPJY-UHFFFAOYSA-N
Formula: C10H15N
SMILES: CCCCc1ccccc1N
Mol. weight [g/mol]: 149.23
CAS: 2696-85-7

Physical Properties

Property code	Value	Unit	Source
gf	202.55	kJ/mol	Joback Method
hf	9.12	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	51.43	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.611		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
ripol	2076.00		NIST Webbook
ripol	2076.00		NIST Webbook
tb	532.39	K	Joback Method
tc	749.29	K	Joback Method
tf	324.66	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.19	J/mol×K	532.39	Joback Method
cpg	330.82	J/mol×K	568.54	Joback Method
cpg	344.61	J/mol×K	604.69	Joback Method
cpg	357.59	J/mol×K	640.84	Joback Method
cpg	369.79	J/mol×K	676.99	Joback Method

cpg	381.24	J/mol×K	713.14	Joback Method
cpg	391.97	J/mol×K	749.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2696857&Units=SI
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume