2-Aminoacetanilide, N-propyl-N'-butyl

Inchi: InChI=1S/C15H24N2O/c1-4-6-11-16-14-9-7-8-10-15(14)17(12-5-2)13(3)18/h7-10,16H,4-
InchiKey: QOMVYJXUBOJUGH-UHFFFAOYSA-N
Formula: C15H24N2O
SMILES: CCCCNc1ccccc1N(CCC)C(C)=O
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	249.45	kJ/mol	Joback Method
hf	-119.45	kJ/mol	Joback Method
hfus	37.98	kJ/mol	Joback Method
hvap	67.15	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.661		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	1872.00		NIST Webbook
rinpol	1872.00		NIST Webbook
tb	690.74	K	Joback Method
tc	889.16	K	Joback Method
tf	432.81	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.63	J/mol×K	690.74	Joback Method
cpg	631.21	J/mol×K	723.81	Joback Method
cpg	646.81	J/mol×K	756.88	Joback Method
cpg	661.47	J/mol×K	789.95	Joback Method
cpg	675.23	J/mol×K	823.02	Joback Method
cpg	688.15	J/mol×K	856.09	Joback Method
cpg	700.26	J/mol×K	889.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R548786&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume