2-Aminoacetanilide, N-propyl-N'-(1-methylpropyl)

Inchi: InChI=1S/C15H24N2O/c1-5-11-17(13(4)18)15-10-8-7-9-14(15)16-12(3)6-2/h7-10,12,16H

InchiKey: CNDYOTOJBYZCIP-UHFFFAOYSA-N

Formula: C15H24N2O

SMILES: CCCN(C(C)=O)c1ccccc1NC(C)CC

Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	247.01	kJ/mol	Joback Method
hf	-124.73	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	66.76	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.660		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	1832.00		NIST Webbook
rinpol	1824.00		NIST Webbook
rinpol	1824.00		NIST Webbook
tb	690.30	K	Joback Method
tc	892.01	K	Joback Method
tf	417.81	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.12	J/mol×K	690.30	Joback Method
cpg	632.00	J/mol×K	723.92	Joback Method
cpg	647.86	J/mol×K	757.54	Joback Method
cpg	662.74	J/mol×K	791.15	Joback Method
cpg	676.68	J/mol×K	824.77	Joback Method
cpg	689.74	J/mol×K	858.39	Joback Method
cpg	701.96	J/mol×K	892.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R548711&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