

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

Inchi:	InChI=1S/C15H24N2O/c1-6-11-17(12(2)18)14-10-8-7-9-13(14)16-15(3,4)5/h7-10,16H,6,
InchiKey:	VMQKPNYFFPHREL-UHFFFAOYSA-N
Formula:	C15H24N2O
SMILES:	CCCN(C(C)=O)c1ccccc1NC(C)(C)C
Mol. weight [g/mol]:	248.36

Physical Properties

Property code	Value	Unit	Source
gf	252.29	kJ/mol	Joback Method
hf	-128.20	kJ/mol	Joback Method
hfus	30.56	kJ/mol	Joback Method
hvap	65.85	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.660		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	1749.00		NIST Webbook
tb	687.51	K	Joback Method
tc	895.60	K	Joback Method
tf	435.23	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.16	J/molxK	687.51	Joback Method
cpg	634.31	J/molxK	722.19	Joback Method
cpg	650.34	J/molxK	756.87	Joback Method
cpg	665.31	J/molxK	791.55	Joback Method
cpg	679.30	J/molxK	826.23	Joback Method
cpg	692.37	J/molxK	860.92	Joback Method
cpg	704.60	J/molxK	895.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R548771&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

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
mccvol:	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

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