

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

Inchi:	InChI=1S/C14H22N2O/c1-5-11(3)15-13-9-7-8-10-14(13)16(6-2)12(4)17/h7-11,15H,5-6H2
InchiKey:	AWXPBZKHTUZNBM-UHFFFAOYSA-N
Formula:	C14H22N2O
SMILES:	CCC(C)Nc1ccccc1N(CC)C(C)=O
Mol. weight [g/mol]:	234.34

Physical Properties

Property code	Value	Unit	Source
gf	238.59	kJ/mol	Joback Method
hf	-104.09	kJ/mol	Joback Method
hfus	31.86	kJ/mol	Joback Method
hvap	64.53	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.270		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1745.00		NIST Webbook
rinpol	1745.00		NIST Webbook
tb	667.42	K	Joback Method
tc	871.66	K	Joback Method
tf	406.54	K	Joback Method
vc	0.764	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.21	J/mol×K	667.42	Joback Method
cpg	577.77	J/mol×K	701.46	Joback Method
cpg	593.31	J/mol×K	735.50	Joback Method
cpg	607.88	J/mol×K	769.54	Joback Method
cpg	621.52	J/mol×K	803.58	Joback Method
cpg	634.28	J/mol×K	837.62	Joback Method
cpg	646.22	J/mol×K	871.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R548746&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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