2-Aminoacetanilide, N,N'-diisobutyl

Inchi: InChI=1S/C16H26N2O/c1-12(2)10-17-15-8-6-7-9-16(15)18(14(5)19)11-13(3)4/h6-9,12-13
InchiKey: VFSWNVWNVUREFA-UHFFFAOYSA-N
Formula: C16H26N2O
SMILES: CC(=O)N(CC(C)C)c1ccccc1NCC(C)C
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	252.99	kJ/mol	Joback Method
hf	-150.65	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	68.60	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.763		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1868.00		NIST Webbook
tb	712.74	K	Joback Method
tc	915.47	K	Joback Method
tf	414.08	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.71	J/mol×K	712.74	Joback Method
cpg	688.17	J/mol×K	746.53	Joback Method
cpg	704.55	J/mol×K	780.32	Joback Method
cpg	719.90	J/mol×K	814.11	Joback Method
cpg	734.27	J/mol×K	847.90	Joback Method
cpg	747.72	J/mol×K	881.69	Joback Method
cpg	760.29	J/mol×K	915.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R548766&Units=SI

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