3-Anilino-2,2,4,4-tetramethyl cyclobutanol

Inchi: InChI=1S/C14H21NO/c1-13(2)11(14(3,4)12(13)16)15-10-8-6-5-7-9-10/h5-9,11-12,15-16H
InchiKey: JPNOFLCISAIPAL-UHFFFAOYSA-N
Formula: C14H21NO
SMILES: CC1(C)C(O)C(C)(C)C1Nc1ccccc1
Mol. weight [g/mol]: 219.32
CAS: 1445-32-5

Physical Properties

Property code	Value	Unit	Source
gf	146.52	kJ/mol	Joback Method
hf	-158.42	kJ/mol	Joback Method
hfus	21.90	kJ/mol	Joback Method
hvap	69.00	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.894		Crippen Method
mcvol	189.350	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
tb	686.23	K	Joback Method
tc	900.73	K	Joback Method
tf	436.94	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.85	J/mol×K	686.23	Joback Method
cpg	567.62	J/mol×K	721.98	Joback Method
cpg	583.81	J/mol×K	757.73	Joback Method
cpg	599.64	J/mol×K	793.48	Joback Method
cpg	615.32	J/mol×K	829.23	Joback Method
cpg	631.06	J/mol×K	864.98	Joback Method
cpg	647.07	J/mol×K	900.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1445325&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume