Aniline,2-methyl-n-(alpha,alpha-dimethylpropyl)-

Inchi: InChI=1S/C12H19N/c1-5-12(3,4)13-11-9-7-6-8-10(11)2/h6-9,13H,5H2,1-4H3
InchiKey: KRBPTYGBTWNJIR-UHFFFAOYSA-N
Formula: C12H19N
SMILES: CCC(C)(C)Nc1ccccc1C
Mol. weight [g/mol]: 177.29

Physical Properties

Property code	Value	Unit	Source
gf	245.17	kJ/mol	Joback Method
hf	-21.23	kJ/mol	Joback Method
hfus	18.17	kJ/mol	Joback Method
hvap	50.38	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.596		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
tb	552.56	K	Joback Method
tc	766.43	K	Joback Method
tf	319.02	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.70	J/mol×K	552.56	Joback Method
cpg	419.13	J/mol×K	588.20	Joback Method
cpg	435.45	J/mol×K	623.85	Joback Method
cpg	450.73	J/mol×K	659.49	Joback Method
cpg	465.02	J/mol×K	695.14	Joback Method
cpg	478.37	J/mol×K	730.78	Joback Method
cpg	490.86	J/mol×K	766.43	Joback Method

Sources

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=B6009279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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