P-tert. amyl aniline

Inchi: InChI=1S/C11H17N/c1-4-11(2,3)9-5-7-10(12)8-6-9/h5-8H,4,12H2,1-3H3
InchiKey: RQUPXQYTWVIBIV-UHFFFAOYSA-N
Formula: C11H17N
SMILES: CCC(C)(C)c1ccc(N)cc1
Mol. weight [g/mol]: 163.26
CAS: 2049-92-5

Physical Properties

Property code	Value	Unit	Source
gf	213.81	kJ/mol	Joback Method
hf	-20.27	kJ/mol	Joback Method
hfus	15.68	kJ/mol	Joback Method
hvap	52.36	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.956		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	552.04	K	Joback Method
tc	779.02	K	Joback Method
tf	338.35	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.95	J/mol×K	552.04	Joback Method
cpg	382.44	J/mol×K	589.87	Joback Method
cpg	397.81	J/mol×K	627.70	Joback Method
cpg	412.11	J/mol×K	665.53	Joback Method
cpg	425.41	J/mol×K	703.36	Joback Method
cpg	437.79	J/mol×K	741.19	Joback Method
cpg	449.30	J/mol×K	779.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2049925&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume