N-n-amyl-p-toluidine

Inchi: InChI=1S/C12H19N/c1-3-4-5-10-13-12-8-6-11(2)7-9-12/h6-9,13H,3-5,10H2,1-2H3
InchiKey: VDOVPACVUJTIMZ-UHFFFAOYSA-N
Formula: C12H19N
SMILES: CCCCCNc1ccc(C)cc1
Mol. weight [g/mol]: 177.29
CAS: 5417-68-5

Physical Properties

Property code	Value	Unit	Source
gf	242.33	kJ/mol	Joback Method
hf	-12.48	kJ/mol	Joback Method
hfus	25.59	kJ/mol	Joback Method
hvap	51.68	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.597		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
tb	555.79	K	Joback Method
tc	757.23	K	Joback Method
tf	316.60	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.59	J/mol×K	555.79	Joback Method
cpg	414.94	J/mol×K	589.36	Joback Method
cpg	430.42	J/mol×K	622.94	Joback Method
cpg	445.05	J/mol×K	656.51	Joback Method
cpg	458.87	J/mol×K	690.08	Joback Method
cpg	471.90	J/mol×K	723.66	Joback Method
cpg	484.19	J/mol×K	757.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5417685&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