O-acetotoluidine, 4-tert-butyl-

Inchi: InChI=1S/C13H19NO/c1-9-8-11(13(3,4)5)6-7-12(9)14-10(2)15/h6-8H,1-5H3,(H,14,15)
InchiKey: CMHOMMAECGTLRB-UHFFFAOYSA-N
Formula: C13H19NO
SMILES: CC(=O)Nc1ccc(C(C)(C)C)cc1C
Mol. weight [g/mol]: 205.30
CAS: 337471-08-6

Physical Properties

Property code	Value	Unit	Source
gf	115.04	kJ/mol	Joback Method
hf	-165.92	kJ/mol	Joback Method
hfus	21.97	kJ/mol	Joback Method
hvap	60.02	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.251		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
tb	634.29	K	Joback Method
tc	852.83	K	Joback Method
tf	392.74	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.54	J/mol×K	634.29	Joback Method
cpg	488.57	J/mol×K	670.71	Joback Method
cpg	503.56	J/mol×K	707.14	Joback Method
cpg	517.55	J/mol×K	743.56	Joback Method
cpg	530.61	J/mol×K	779.99	Joback Method
cpg	542.79	J/mol×K	816.41	Joback Method
cpg	554.15	J/mol×K	852.83	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=C337471086&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume