2,6-Diethyl-m-toluidine

Inchi: InChI=1S/C11H17N/c1-4-9-7-6-8(3)10(5-2)11(9)12/h6-7H,4-5,12H2,1-3H3
InchiKey: OXYMEFWXAVMOEB-UHFFFAOYSA-N
Formula: C11H17N
SMILES: CCc1ccc(C)c(CC)c1N
Mol. weight [g/mol]: 163.26
CAS: 67330-61-4

Physical Properties

Property code	Value	Unit	Source
gf	191.71	kJ/mol	Joback Method
hf	-34.46	kJ/mol	Joback Method
hfus	22.32	kJ/mol	Joback Method
hvap	54.98	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.702		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	1397.00		NIST Webbook
tb	565.23	K	Joback Method
tc	780.61	K	Joback Method
tf	360.97	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.28	J/mol×K	565.23	Joback Method
cpg	377.14	J/mol×K	601.13	Joback Method
cpg	391.22	J/mol×K	637.02	Joback Method
cpg	404.55	J/mol×K	672.92	Joback Method
cpg	417.15	J/mol×K	708.82	Joback Method
cpg	429.04	J/mol×K	744.71	Joback Method
cpg	440.24	J/mol×K	780.61	Joback Method

Sources

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=C67330614&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume