3-(o-Toluidino)-1-propanol

Inchi: InChI=1S/C9H13NO/c10-9-6-2-1-4-8(9)5-3-7-11/h1-2,4,6,11H,3,5,7,10H2
InchiKey: DXAZQYFSQMFTIP-UHFFFAOYSA-N
Formula: C9H13NO
SMILES: Nc1ccccc1CCCO
Mol. weight [g/mol]: 151.21

Physical Properties

Property code	Value	Unit	Source
gf	57.31	kJ/mol	Joback Method
hf	-122.47	kJ/mol	Joback Method
hfus	22.00	kJ/mol	Joback Method
hvap	65.89	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.194		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
rinpol	1451.00		NIST Webbook
tb	601.69	K	Joback Method
tc	806.50	K	Joback Method
tf	374.21	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.22	J/mol×K	601.69	Joback Method
cpg	332.40	J/mol×K	635.83	Joback Method
cpg	342.93	J/mol×K	669.96	Joback Method
cpg	352.84	J/mol×K	704.10	Joback Method
cpg	362.15	J/mol×K	738.23	Joback Method
cpg	370.89	J/mol×K	772.37	Joback Method
cpg	379.10	J/mol×K	806.50	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=R264790&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume