3-Toluoylacetonitrile

Inchi: InChI=1S/C10H9NO/c1-8-3-2-4-9(7-8)10(12)5-6-11/h2-4,7H,5H2,1H3
InchiKey: IVLKDYOTZMFMLO-UHFFFAOYSA-N
Formula: C10H9NO
SMILES: Cc1cccc(C(=O)CC#N)c1
Mol. weight [g/mol]: 159.18
CAS: 53882-81-8

Physical Properties

Property code	Value	Unit	Source
gf	140.36	kJ/mol	Joback Method
hf	27.63	kJ/mol	Joback Method
hfus	18.41	kJ/mol	Joback Method
hvap	58.02	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.091		Crippen Method
mcvol	130.950	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
tb	615.81	K	Joback Method
tc	847.63	K	Joback Method
tf	356.32	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.20	J/mol×K	615.81	Joback Method
cpg	311.13	J/mol×K	654.45	Joback Method
cpg	321.30	J/mol×K	693.08	Joback Method
cpg	330.75	J/mol×K	731.72	Joback Method
cpg	339.51	J/mol×K	770.36	Joback Method
cpg	347.62	J/mol×K	809.00	Joback Method
cpg	355.11	J/mol×K	847.63	Joback Method

Sources

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=C53882818&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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