2,4,5-Trimethylphenylacetonitrile

Inchi: InChI=1S/C11H13N/c1-8-6-10(3)11(4-5-12)7-9(8)2/h6-7H,4H2,1-3H3
InchiKey: MSZOPWWSWGLPST-UHFFFAOYSA-N
Formula: C11H13N
SMILES: Cc1cc(C)c(CC#N)cc1C
Mol. weight [g/mol]: 159.23
CAS: 75279-58-2

Physical Properties

Property code	Value	Unit	Source
gf	258.44	kJ/mol	Joback Method
hf	96.63	kJ/mol	Joback Method
hfus	18.63	kJ/mol	Joback Method
hvap	54.82	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.678		Crippen Method
mcvol	143.470	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
tb	594.78	K	Joback Method
tc	817.07	K	Joback Method
tf	342.70	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.16	J/mol×K	594.78	Joback Method
cpg	344.77	J/mol×K	631.83	Joback Method
cpg	356.69	J/mol×K	668.88	Joback Method
cpg	367.93	J/mol×K	705.92	Joback Method
cpg	378.53	J/mol×K	742.97	Joback Method
cpg	388.49	J/mol×K	780.02	Joback Method
cpg	397.84	J/mol×K	817.07	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=C75279582&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