2,5-Dimethyl-4-methoxyphenylacetonitrile

Inchi: InChI=1S/C11H13NO/c1-8-7-11(13-3)9(2)6-10(8)4-5-12/h6-7H,4H2,1-3H3
InchiKey: XPKNQRIEXCGMHA-UHFFFAOYSA-N
Formula: C11H13NO
SMILES: COc1cc(C)c(CC#N)cc1C
Mol. weight [g/mol]: 175.23
CAS: 105909-12-4

Physical Properties

Property code	Value	Unit	Source
gf	153.44	kJ/mol	Joback Method
hf	-35.59	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	57.23	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.378		Crippen Method
mcvol	149.340	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
tb	617.20	K	Joback Method
tc	836.68	K	Joback Method
tf	364.93	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.77	J/mol×K	617.20	Joback Method
cpg	368.23	J/mol×K	653.78	Joback Method
cpg	380.03	J/mol×K	690.36	Joback Method
cpg	391.19	J/mol×K	726.94	Joback Method
cpg	401.69	J/mol×K	763.52	Joback Method
cpg	411.55	J/mol×K	800.10	Joback Method
cpg	420.77	J/mol×K	836.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105909124&Units=SI
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

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