2,3,4-Trimethoxyphenylacetonitrile

Inchi: InChI=1S/C11H13NO3/c1-13-9-5-4-8(6-7-12)10(14-2)11(9)15-3/h4-5H,6H2,1-3H3
InchiKey: RZVUKELRMABJPI-UHFFFAOYSA-N
Formula: C11H13NO3
SMILES: COc1ccc(CC#N)c(OC)c1OC
Mol. weight [g/mol]: 207.23
CAS: 68913-85-9

Physical Properties

Property code	Value	Unit	Source
gf	-56.56	kJ/mol	Joback Method
hf	-300.03	kJ/mol	Joback Method
hfus	22.19	kJ/mol	Joback Method
hvap	62.05	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	1.778		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
tb	662.04	K	Joback Method
tc	876.35	K	Joback Method
tf	409.39	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.77	J/mol×K	662.04	Joback Method
cpg	415.99	J/mol×K	697.76	Joback Method
cpg	427.58	J/mol×K	733.48	Joback Method
cpg	438.51	J/mol×K	769.20	Joback Method
cpg	448.74	J/mol×K	804.91	Joback Method
cpg	458.24	J/mol×K	840.63	Joback Method
cpg	467.00	J/mol×K	876.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68913859&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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