3-Fluoro-4-methoxyphenylacetonitrile

Inchi: InChI=1S/C9H8FNO/c1-12-9-3-2-7(4-5-11)6-8(9)10/h2-3,6H,4H2,1H3
InchiKey: OFCMGCZEFVKTAN-UHFFFAOYSA-N
Formula: C9H8FNO
SMILES: COc1ccc(CC#N)cc1F
Mol. weight [g/mol]: 165.16
CAS: 404-90-0

Physical Properties

Property code	Value	Unit	Source
gf	-48.58	kJ/mol	Joback Method
hf	-178.95	kJ/mol	Joback Method
hfus	18.10	kJ/mol	Joback Method
hvap	51.30	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	1.900		Crippen Method
mcvol	122.930	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
tb	565.73	K	Joback Method
tc	781.30	K	Joback Method
tf	330.46	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.89	J/mol×K	565.73	Joback Method
cpg	283.08	J/mol×K	601.66	Joback Method
cpg	292.74	J/mol×K	637.59	Joback Method
cpg	301.86	J/mol×K	673.52	Joback Method
cpg	310.46	J/mol×K	709.44	Joback Method
cpg	318.53	J/mol×K	745.37	Joback Method
cpg	326.08	J/mol×K	781.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C404900&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