4-Fluoro-2-methoxyphenol

Inchi: InChI=1S/C7H7FO2/c1-10-7-4-5(8)2-3-6(7)9/h2-4,9H,1H3
InchiKey: OULGLTLTWBZBLO-UHFFFAOYSA-N
Formula: C7H7FO2
SMILES: COc1cc(F)ccc1O
Mol. weight [g/mol]: 142.13
CAS: 450-93-1

Physical Properties

Property code	Value	Unit	Source
gf	-343.59	kJ/mol	Joback Method
hf	-468.39	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	48.72	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.540		Crippen Method
mcvol	99.240	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
rinpol	1107.90		NIST Webbook
rinpol	1107.90		NIST Webbook
tb	493.53	K	Joback Method
tc	710.11	K	Joback Method
tf	342.13	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.50	J/mol×K	493.53	Joback Method
cpg	222.98	J/mol×K	529.63	Joback Method
cpg	231.84	J/mol×K	565.72	Joback Method
cpg	240.14	J/mol×K	601.82	Joback Method
cpg	247.92	J/mol×K	637.92	Joback Method
cpg	255.22	J/mol×K	674.01	Joback Method
cpg	262.09	J/mol×K	710.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C450931&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume