Benzene, 1-ethoxy-4-fluoro-

Other names: 4-FLUOROPHENETOLE
Phenetole, p-fluoro-
p-Fluorophenetole
Inchi: InChI=1S/C8H9FO/c1-2-10-8-5-3-7(9)4-6-8/h3-6H,2H2,1H3
InchiKey: PURLWQWDGIIYBG-UHFFFAOYSA-N
Formula: C8H9FO
SMILES: CCOc1ccc(F)cc1
Mol. weight [g/mol]: 140.15
CAS: 459-26-7

Physical Properties

Property code	Value	Unit	Source
chl	-4282.95	kJ/mol	NIST Webbook
gf	-180.55	kJ/mol	Joback Method
hf	-311.72	kJ/mol	Joback Method
hfus	14.40	kJ/mol	Joback Method
hvap	37.93	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.224		Crippen Method
mcvol	107.460	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	445.65	K	KDB
tc	634.28	K	Joback Method
tf	264.65	K	KDB
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.33	J/mol×K	435.79	Joback Method
cpg	218.63	J/mol×K	468.87	Joback Method
cpg	229.42	J/mol×K	501.95	Joback Method
cpg	239.72	J/mol×K	535.04	Joback Method
cpg	249.52	J/mol×K	568.12	Joback Method

cpg	258.84	J/mol×K	601.20	Joback Method
cpg	267.69	J/mol×K	634.28	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1809.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C459267&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
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