3-Fluoro-o-xylene

Other names: 1-Fluoro-2,3-dimethylbenzene
2,3-Dimethylfluorobenzene
3-Fluoro-1,2-xylene
Benzene, 1-fluoro-2,3-dimethyl-
o-Xylene, 3-fluoro-
Inchi: InChI=1S/C8H9F/c1-6-4-3-5-8(9)7(6)2/h3-5H,1-2H3
InchiKey: AWLDSXJCQWTJPC-UHFFFAOYSA-N
Formula: C8H9F
SMILES: Cc1cccc(F)c1C
Mol. weight [g/mol]: 124.16
CAS: 443-82-3

Physical Properties

Property code	Value	Unit	Source
gf	-85.18	kJ/mol	Joback Method
hf	-190.97	kJ/mol	Joback Method
hfus	12.82	kJ/mol	Joback Method
hvap	36.19	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.443		Crippen Method
mcvol	101.590	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
tb	423.20	K	NIST Webbook
tc	619.18	K	Joback Method
tf	231.97	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.01	J/mol×K	418.35	Joback Method
cpg	197.13	J/mol×K	451.82	Joback Method
cpg	207.71	J/mol×K	485.29	Joback Method
cpg	217.79	J/mol×K	518.76	Joback Method

cpg	227.36	J/mol×K	552.23	Joback Method
cpg	236.44	J/mol×K	585.71	Joback Method
cpg	245.06	J/mol×K	619.18	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45466e+01
Coeff. B	-3.61799e+03
Coeff. C	-5.87860e+01
Temperature range (K), min.	312.52
Temperature range (K), max.	450.55

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C443823&Units=SI

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

pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume