

5-Fluoro-m-xylene

Inchi:	InChI=1S/C8H9F/c1-6-3-7(2)5-8(9)4-6/h3-5H,1-2H3
InchiKey:	RCWIWNUVHNAUQC-UHFFFAOYSA-N
Formula:	C8H9F
SMILES:	Cc1cc(C)cc(F)c1
Mol. weight [g/mol]:	124.16
CAS:	461-97-2

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	418.35	K	Joback Method
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/molxK	418.35	Joback Method
cpg	197.13	J/molxK	451.82	Joback Method
cpg	207.71	J/molxK	485.29	Joback Method
cpg	217.79	J/molxK	518.76	Joback Method
cpg	227.36	J/molxK	552.23	Joback Method
cpg	236.44	J/molxK	585.71	Joback Method
cpg	245.06	J/molxK	619.18	Joback Method

Sources

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=C461972&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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