

4-Fluoro-1,2-dimethylbenzene

Inchi: InChI=1S/C8H9F/c1-6-3-4-8(9)5-7(6)2/h3-5H,1-2H3
InchiKey: WYHBENDEZDFJNU-UHFFFAOYSA-N
Formula: C8H9F
SMILES: Cc1ccc(F)cc1C
Mol. weight [g/mol]: 124.16

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
ripol	2211.00		NIST Webbook
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/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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R640956&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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