

2,6-Dimethylfluorobenzene

Other names:	2-Fluoro-1,3-dimethylbenzene 2-Fluoro-m-xylene Benzene, 2-fluoro-1,3-dimethyl-
Inchi:	InChI=1S/C8H9F/c1-6-4-3-5-7(2)8(6)9/h3-5H,1-2H3
InchiKey:	JTAUTNBVFDTYTI-UHFFFAOYSA-N
Formula:	C8H9F
SMILES:	Cc1cccc(C)c1F
Mol. weight [g/mol]:	124.16
CAS:	443-88-9

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/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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46390e+01
Coeff. B	-3.62270e+03
Coeff. C	-5.80910e+01
Temperature range (K), min.	310.52
Temperature range (K), max.	446.48

Sources

The Yaws Handbook of Vapor
Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback Method:

https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method:

https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C443889&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

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