

2,5-DIFLUOROTOLUENE

Other names:	Benzene, 1,4-difluoro-2-methyl-
Inchi:	InChI=1S/C7H6F2/c1-5-4-6(8)2-3-7(5)9/h2-4H,1H3
InchiKey:	YSNVKDGEALPJGC-UHFFFAOYSA-N
Formula:	C7H6F2
SMILES:	Cc1cc(F)ccc1F
Mol. weight [g/mol]:	128.12
CAS:	452-67-5

Physical Properties

Property code	Value	Unit	Source
hf	-340.71	kJ/mol	Cheméo Relay (1.0)
hfus	13.31	kJ/mol	Joback Method
hvap	41.77	kJ/mol	Cheméo Relay (1.0)
ie	8.90	eV	Cheméo Relay (1.0)
logp	2.273		Crippen Method
mcvol	89.270	ml/mol	McGowan Method
tb	390.00	K	NIST Webbook
tc	601.55	K	Cheméo Relay (1.0)
tf	227.27	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.53	J/mol×K	394.74	Joback Method
cpg	166.74	J/mol×K	426.65	Joback Method
cpg	175.52	J/mol×K	458.56	Joback Method
cpg	183.89	J/mol×K	490.47	Joback Method
cpg	191.84	J/mol×K	522.38	Joback Method
cpg	199.40	J/mol×K	554.29	Joback Method
cpg	206.58	J/mol×K	586.20	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.20	K	103.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47467e+01
Coeff. B	-3.44786e+03
Coeff. C	-4.95840e+01
Temperature range (K), min.	288.04
Temperature range (K), max.	415.01

Sources

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

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

Joback Method:

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

McGowan Method:

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

Crippen Method:

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

Crippen Method:

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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