2,4-Difluorotoluene

Other names: Benzene, 2,4-difluoro-1-methyl-
Inchi: InChI=1S/C7H6F2/c1-5-2-3-6(8)4-7(5)9/h2-4H,1H3
InchiKey: MPXDAIBTYWGBSL-UHFFFAOYSA-N
Formula: C7H6F2
SMILES: Cc1ccc(F)cc1F
Mol. weight [g/mol]: 128.12
CAS: 452-76-6

Physical Properties

Property code	Value	Unit	Source
gf	-288.41	kJ/mol	Joback Method
hf	-366.44	kJ/mol	Joback Method
hfus	13.31	kJ/mol	Joback Method
hvap	33.14	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.273		Crippen Method
mcvol	89.270	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
tb	388.20	K	NIST Webbook
tb	387.50 ± 0.50	K	NIST Webbook
tc	586.20	K	Joback Method
tf	221.29	K	Joback Method
vc	0.355	m3/kmol	Joback Method

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47324e+01
Coeff. B	-3.43012e+03
Coeff. C	-4.90560e+01
Temperature range (K), min.	286.52
Temperature range (K), max.	413.15

Sources

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=C452766&Units=SI
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

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