Toluene, «alpha»-fluoro-

Other names: (Fluoromethyl)benzene
Benzyl fluoride
«alpha»-Fluorotoluene
Inchi: InChI=1S/C7H7F/c8-6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey: MBXXQYJBFRRFCK-UHFFFAOYSA-N
Formula: C7H7F
SMILES: FCc1ccccc1
Mol. weight [g/mol]: 110.13
CAS: 25496-08-6

Physical Properties

Property code	Value	Unit	Source
af	0.3169		Cheméo Relay (1.0)
gf	-74.34	kJ/mol	Joback Method
hf	-145.91	kJ/mol	Cheméo Relay (1.0)
hfus	11.01	kJ/mol	Joback Method
hvap	42.07	kJ/mol	Cheméo Relay (1.0)
ie	9.36	eV	Cheméo Relay (1.0)
log10ws	-1.74		Cheméo Relay (1.0)
logp	2.156		Crippen Method
mcvol	87.500	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
tb	408.98	K	Cheméo Relay (1.0)
tc	623.91	K	Cheméo Relay (1.0)
tf	233.55	K	Cheméo Relay (1.0)
vc	0.323	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.45	J/mol×K	385.51	Joback Method
cpg	157.30	J/mol×K	418.75	Joback Method
cpg	167.55	J/mol×K	451.99	Joback Method
cpg	177.20	J/mol×K	485.23	Joback Method

cpg	186.30	J/mol×K	518.48	Joback Method
cpg	194.85	J/mol×K	551.72	Joback Method
cpg	202.89	J/mol×K	584.96	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46318e+01
Coeff. B	-3.56474e+03
Coeff. C	-5.60060e+01
Temperature range (K), min.	304.52
Temperature range (K), max.	438.48

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25496086&Units=SI
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

af: Acentric Factor
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
ie: Ionization energy

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