2-fluoro-1-phenylethanone

Inchi: InChI=1S/C8H7FO/c9-6-8(10)7-4-2-1-3-5-7/h1-5H,6H2
InchiKey: YOMBUJAFGMOIGS-UHFFFAOYSA-N
Formula: C8H7FO
SMILES: O=C(CF)c1ccccc1
Mol. weight [g/mol]: 138.14
CAS: 450-95-3

Physical Properties

Property code	Value	Unit	Source
af	0.4215		Cheméo Relay (1.0)
gf	-194.84	kJ/mol	Joback Method
hf	-269.92	kJ/mol	Cheméo Relay (1.0)
hfus	15.20	kJ/mol	Joback Method
hvap	57.05	kJ/mol	Cheméo Relay (1.0)
ie	9.48	eV	Cheméo Relay (1.0)
log10ws	-1.69		Cheméo Relay (1.0)
logp	1.839		Crippen Method
mcvol	103.160	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
tb	481.76	K	Cheméo Relay (1.0)
tc	697.64	K	Cheméo Relay (1.0)
tf	302.21	K	Cheméo Relay (1.0)
vc	0.375	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.67	J/mol×K	462.26	Joback Method
cpg	211.84	J/mol×K	497.23	Joback Method
cpg	222.32	J/mol×K	532.21	Joback Method
cpg	232.14	J/mol×K	567.18	Joback Method
cpg	241.33	J/mol×K	602.16	Joback Method
cpg	249.91	J/mol×K	637.13	Joback Method
cpg	257.90	J/mol×K	672.10	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.03858e+01
Coeff. B	-7.45209e+03
Temperature range (K), min.	370.78
Temperature range (K), max.	494.36

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: 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

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