3-FLUOROSTYRENE

Other names: m-Fluorostyrene
3-Fluorostyrene
Inchi: InChI=1S/C8H7F/c1-2-7-4-3-5-8(9)6-7/h2-6H,1H2
InchiKey: ZJSKEGAHBAHFON-UHFFFAOYSA-N
Formula: C8H7F
SMILES: C=Cc1cccc(F)c1
Mol. weight [g/mol]: 122.14

Physical Properties

Property code	Value	Unit	Source
af	0.2861		Cheméo Relay (1.0)
hf	-62.41	kJ/mol	Cheméo Relay (1.0)
hfus	11.93	kJ/mol	Joback Method
hvap	44.00	kJ/mol	Cheméo Relay (1.0)
ie	8.76	eV	Cheméo Relay (1.0)
log10ws	-2.33		Cheméo Relay (1.0)
logp	2.469		Crippen Method
mcvol	97.290	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	415.13	K	Cheméo Relay (1.0)
tc	626.54	K	Cheméo Relay (1.0)
tf	205.38	K	Cheméo Relay (1.0)
vc	0.358	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.86	J/mol×K	410.05	Joback Method
cpg	180.79	J/mol×K	444.02	Joback Method
cpg	191.09	J/mol×K	477.99	Joback Method
cpg	200.80	J/mol×K	511.96	Joback Method
cpg	209.92	J/mol×K	545.94	Joback Method
cpg	218.50	J/mol×K	579.91	Joback Method
cpg	226.55	J/mol×K	613.88	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	303.70	K	0.50	NIST Webbook

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C350516&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume