Benzene, 1-(chloromethyl)-4-fluoro-

Other names:	1-(Chloromethyl)-4-fluorobenzene 4-Fluorobenzyl chloride Toluene, «alpha»-chloro-p-fluoro- Toluene, Â«alphaÂ»-chloro-p-fluoro- p-Fluorobenzyl chloride «alpha»-Chloro-4-fluorotoluene «alpha»-Chloro-p-fluorotoluene Â«alphaÂ»-Chloro-4-fluorotoluene Â«alphaÂ»-Chloro-p-fluorotoluene
Inchi:	InChI=1S/C7H6ClF/c8-5-6-1-3-7(9)4-2-6/h1-4H,5H2
InchiKey:	IZXWCDITFDNEBY-UHFFFAOYSA-N
Formula:	C7H6ClF
SMILES:	Fc1ccc(CCl)cc1
Mol. weight [g/mol]:	144.57
CAS:	352-11-4

Physical Properties

Property code	Value	Unit	Source
gf	-95.90	kJ/mol	Joback Method
hf	-174.60	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	37.68	kJ/mol	Joback Method
log10ws	-2.54		Aqueous Solubility Prediction Method
logp	2.564		Crippen Method
mcvol	99.740	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	989.60		NIST Webbook
rinpol	989.60		NIST Webbook
tb	427.92	K	Joback Method
tc	636.83	K	Joback Method
tf	238.10	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.12	J/mol×K	427.92	Joback Method
cpg	181.95	J/mol×K	462.74	Joback Method
cpg	191.20	J/mol×K	497.56	Joback Method
cpg	199.89	J/mol×K	532.38	Joback Method
cpg	208.06	J/mol×K	567.20	Joback Method
cpg	215.72	J/mol×K	602.01	Joback Method
cpg	222.90	J/mol×K	636.83	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.50 ± 0.50	K	4.00	NIST Webbook
tbrp	355.20	K	3.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C352114&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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