

Benzene, 1-(chloromethyl)-3-fluoro-

Other names:	Toluene, «alpha»-chloro-m-fluoro- «alpha»-Chloro-m-fluorotoluene «alpha»-Chloro-3-fluorotoluene m-Fluorobenzyl chloride 1-(Chloromethyl)-3-fluorobenzene 3-Fluorobenzyl chloride 3-Fluorophenylmethyl chloride «alpha»-chloro-p-fluorotoluene
Inchi:	InChI=1S/C7H6ClF/c8-5-6-2-1-3-7(9)4-6/h1-4H,5H2
InchiKey:	XBDXMDVEZLOGMC-UHFFFAOYSA-N
Formula:	C7H6ClF
SMILES:	Fc1cccc(CCl)c1
Mol. weight [g/mol]:	144.57
CAS:	456-42-8

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	-2.84		Crippen Method
logp	2.564		Crippen Method
mcvol	99.740	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	987.10		NIST Webbook
rinpol	987.10		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	987.10		NIST Webbook
tb	427.92	K	Joback Method
tc	636.83	K	Joback Method
tf	238.10	K	Joback Method
vc	0.387	m ³ /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

Sources

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=C456428&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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