

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

Other names:	«alpha»'-Chloro-«alpha», «alpha», «alpha»-trifluoro-m-xylene 3-Trifluoromethylbenzyl chloride m-Trifluoromethylbenzyl chloride 3-Chloromethylbenzotrifluoride «alpha»-Chloro-3-trifluoromethyltoluene m-Xylene, «alpha»'-chloro-«alpha», «alpha», «alpha»-trifluoro-1-(Chloromethyl)-3-(trifluoromethyl)benzene NSC 5227
Inchi:	InChI=1S/C8H6ClF3/c9-5-6-2-1-3-7(4-6)8(10,11)12/h1-4H,5H2
InchiKey:	XGASTRVQNVVYIZ-UHFFFAOYSA-N
Formula:	C8H6ClF3
SMILES:	FC(F)(F)c1cccc(CCl)c1
Mol. weight [g/mol]:	194.58
CAS:	705-29-3

Physical Properties

Property code	Value	Unit	Source
gf	-474.26	kJ/mol	Joback Method
hf	-596.21	kJ/mol	Joback Method
hfus	16.15	kJ/mol	Joback Method
hvap	36.98	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.444		Crippen Method
mcvol	117.370	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	446.11	K	Joback Method
tc	643.63	K	Joback Method
tf	252.97	K	Joback Method
vc	0.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.05	J/mol×K	446.11	Joback Method

cpg	241.23	J/mol×K	479.03	Joback Method
cpg	251.64	J/mol×K	511.95	Joback Method
cpg	261.33	J/mol×K	544.87	Joback Method
cpg	270.32	J/mol×K	577.79	Joback Method
cpg	278.66	J/mol×K	610.71	Joback Method
cpg	286.38	J/mol×K	643.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	342.00 ± 1.00	K	1.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C705293&Units=SI

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
mccvol:	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

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