3,5-Bis(trifluoromethyl)benzyl chloride

Other names:	3,5-di(Trifluoromethyl)benzyl chloride
	Benzene, 1-(chloromethyl)-3,5-bis(trifluoromethyl)-
	1-(chloromethyl)-3,5-bis(trifluoromethyl)benzene
Inchi:	InChI=1S/C9H5ClF6/c10-4-5-1-6(8(11,12)13)3-7(2-5)9(14,15)16/h1-3H,4H2
InchiKey:	OINTXXMBRBLMHH-UHFFFAOYSA-N
Formula:	C9H5ClF6
SMILES:	FC(F)(F)c1cc(CCl)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	262.58
CAS:	75462-59-8

Physical Properties

Property code	Value	Unit	Source
gf	-1057.06	kJ/mol	Joback Method
hf	-1225.40	kJ/mol	Joback Method
hfus	20.18	kJ/mol	Joback Method
hvap	36.12	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.463		Crippen Method
mcvol	136.770	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
tb	468.55	K	Joback Method
tc	647.69	K	Joback Method
tf	280.95	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.15	J/mol×K	468.55	Joback Method
cpg	310.29	J/mol×K	498.41	Joback Method
cpg	320.64	J/mol×K	528.26	Joback Method
cpg	330.25	J/mol×K	558.12	Joback Method
cpg	339.16	J/mol×K	587.98	Joback Method
cpg	347.41	J/mol×K	617.83	Joback Method

cpg	355.05	J/mol×K	647.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C75462598&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume