Benzene, 1-chloro-3-trifluoroacetyl

Inchi: InChI=1S/C8H4ClF3O/c9-6-3-1-2-5(4-6)7(13)8(10,11)12/h1-4H
InchiKey: KYFMLRJTDPGABF-UHFFFAOYSA-N
Formula: C8H4ClF3O
SMILES: O=C(c1cccc(Cl)c1)C(F)(F)F
Mol. weight [g/mol]: 208.56

Physical Properties

Property code	Value	Unit	Source
gf	-603.18	kJ/mol	Joback Method
hf	-708.79	kJ/mol	Joback Method
hfus	17.75	kJ/mol	Joback Method
hvap	43.72	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.085		Crippen Method
mcvol	118.940	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1012.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1012.00		NIST Webbook
tb	499.98	K	Joback Method
tc	708.00	K	Joback Method
tf	302.90	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.85	J/mol×K	499.98	Joback Method
cpg	254.75	J/mol×K	534.65	Joback Method
cpg	263.88	J/mol×K	569.32	Joback Method
cpg	272.28	J/mol×K	603.99	Joback Method
cpg	280.00	J/mol×K	638.66	Joback Method
cpg	287.08	J/mol×K	673.33	Joback Method
cpg	293.57	J/mol×K	708.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R345443&Units=SI
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

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