Benzene, 1-methoxy-4-(1-chloro-2,2,2-trifluoroethyl)

Inchi: InChI=1S/C9H8ClF3O/c1-14-7-4-2-6(3-5-7)8(10)9(11,12)13/h2-5,8H,1H3
InchiKey: YLITYVXPYIDNLA-UHFFFAOYSA-N
Formula: C9H8ClF3O
SMILES: COc1ccc(C(Cl)C(F)(F)F)cc1
Mol. weight [g/mol]: 224.61

Physical Properties

Property code	Value	Unit	Source
gf	-573.28	kJ/mol	Joback Method
hf	-754.35	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hvap	41.23	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.537		Crippen Method
mcvol	137.330	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	1202.00		NIST Webbook
rinpol	1202.00		NIST Webbook
tb	490.97	K	Joback Method
tc	689.29	K	Joback Method
tf	271.47	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.26	J/mol×K	490.97	Joback Method
cpg	306.37	J/mol×K	524.02	Joback Method
cpg	317.73	J/mol×K	557.08	Joback Method
cpg	328.36	J/mol×K	590.13	Joback Method
cpg	338.30	J/mol×K	623.18	Joback Method
cpg	347.58	J/mol×K	656.24	Joback Method
cpg	356.22	J/mol×K	689.29	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=R515132&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume