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

Inchi: InChI=1S/C9H7Cl2F3O/c1-15-7-4-2-6(3-5-7)8(10,11)9(12,13)14/h2-5H,1H3
InchiKey: ABMVKEFNQCDUJN-UHFFFAOYSA-N
Formula: C9H7Cl2F3O
SMILES: COc1ccc(C(Cl)(Cl)C(F)(F)F)cc1
Mol. weight [g/mol]: 259.05

Physical Properties

Property code	Value	Unit	Source
gf	-579.93	kJ/mol	Joback Method
hf	-773.56	kJ/mol	Joback Method
hfus	16.71	kJ/mol	Joback Method
hvap	44.70	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.888		Crippen Method
mcvol	149.570	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1478.00		NIST Webbook
tb	525.61	K	Joback Method
tc	737.39	K	Joback Method
tf	318.81	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.23	J/mol×K	525.61	Joback Method
cpg	335.07	J/mol×K	560.91	Joback Method
cpg	345.95	J/mol×K	596.20	Joback Method
cpg	355.94	J/mol×K	631.50	Joback Method
cpg	365.09	J/mol×K	666.80	Joback Method
cpg	373.47	J/mol×K	702.09	Joback Method
cpg	381.13	J/mol×K	737.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515127&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