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

Inchi: InChI=1S/C9H9F3O/c1-13-8-4-2-7(3-5-8)6-9(10,11)12/h2-5H,6H2,1H3
InchiKey: RCMJDIMTNJVPAN-UHFFFAOYSA-N
Formula: C9H9F3O
SMILES: COc1ccc(CC(F)(F)F)cc1
Mol. weight [g/mol]: 190.16

Physical Properties

Property code	Value	Unit	Source
gf	-558.91	kJ/mol	Joback Method
hf	-733.33	kJ/mol	Joback Method
hfus	15.73	kJ/mol	Joback Method
hvap	37.23	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.800		Crippen Method
mcvol	125.090	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	1052.00		NIST Webbook
rinpol	1052.00		NIST Webbook
tb	453.98	K	Joback Method
tc	642.08	K	Joback Method
tf	256.55	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.86	J/mol×K	453.98	Joback Method
cpg	279.33	J/mol×K	485.33	Joback Method
cpg	291.10	J/mol×K	516.68	Joback Method
cpg	302.21	J/mol×K	548.03	Joback Method
cpg	312.68	J/mol×K	579.38	Joback Method
cpg	322.54	J/mol×K	610.73	Joback Method
cpg	331.80	J/mol×K	642.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515023&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