Benzene, 1-trifluoromethyl-3-(2,2,2-trifluoroethyl)

Inchi: InChI=1S/C9H6F6/c10-8(11,12)5-6-2-1-3-7(4-6)9(13,14)15/h1-4H,5H2
InchiKey: ZDMPOTKYTHEWOD-UHFFFAOYSA-N
Formula: C9H6F6
SMILES: FC(F)(F)Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 228.13

Physical Properties

Property code	Value	Unit	Source
gf	-1035.50	kJ/mol	Joback Method
hf	-1198.19	kJ/mol	Joback Method
hfus	16.37	kJ/mol	Joback Method
hvap	31.07	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.810		Crippen Method
mcvol	124.530	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
tb	426.14	K	Joback Method
tc	597.68	K	Joback Method
tf	238.51	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.93	J/mol×K	426.14	Joback Method
cpg	282.34	J/mol×K	454.73	Joback Method
cpg	293.94	J/mol×K	483.32	Joback Method
cpg	304.76	J/mol×K	511.91	Joback Method
cpg	314.85	J/mol×K	540.50	Joback Method
cpg	324.23	J/mol×K	569.09	Joback Method
cpg	332.96	J/mol×K	597.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R345423&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