Benzene, (2,2,2-trifluoroethyl)

Inchi: InChI=1S/C8H7F3/c9-8(10,11)6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey: AVSVJSGDSPDFLH-UHFFFAOYSA-N
Formula: C8H7F3
SMILES: FC(F)(F)Cc1ccccc1
Mol. weight [g/mol]: 160.14

Physical Properties

Property code	Value	Unit	Source
gf	-452.70	kJ/mol	Joback Method
hf	-569.00	kJ/mol	Joback Method
hfus	12.34	kJ/mol	Joback Method
hvap	31.93	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.791		Crippen Method
mcvol	105.130	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	812.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	812.00		NIST Webbook
tb	403.70	K	Joback Method
tc	592.66	K	Joback Method
tf	210.53	K	Joback Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.97	J/mol×K	403.70	Joback Method
cpg	214.38	J/mol×K	435.19	Joback Method
cpg	225.99	J/mol×K	466.69	Joback Method
cpg	236.83	J/mol×K	498.18	Joback Method
cpg	246.95	J/mol×K	529.68	Joback Method
cpg	256.37	J/mol×K	561.17	Joback Method
cpg	265.13	J/mol×K	592.66	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=R345438&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