1-Phenyl-2,2,2-trifluoroethanol

Other names: Benzeneethanol, «alpha»-trifluoromethyl
Inchi: InChI=1S/C8H7F3O/c9-8(10,11)7(12)6-4-2-1-3-5-6/h1-5,7,12H
InchiKey: VNOMEAQPOMDWSR-UHFFFAOYSA-N
Formula: C8H7F3O
SMILES: OC(c1ccccc1)C(F)(F)F
Mol. weight [g/mol]: 176.14
CAS: 340-04-5

Physical Properties

Property code	Value	Unit	Source
gf	-591.96	kJ/mol	Joback Method
hf	-726.51	kJ/mol	Joback Method
hfus	12.91	kJ/mol	Joback Method
hvap	48.22	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.282		Crippen Method
mcvol	111.000	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
rinpol	1054.00		NIST Webbook
tb	495.44	K	Joback Method
tc	679.83	K	Joback Method
tf	256.35	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.18	J/mol×K	495.44	Joback Method
cpg	262.51	J/mol×K	526.17	Joback Method
cpg	272.14	J/mol×K	556.90	Joback Method
cpg	281.12	J/mol×K	587.63	Joback Method
cpg	289.46	J/mol×K	618.36	Joback Method
cpg	297.22	J/mol×K	649.09	Joback Method
cpg	304.42	J/mol×K	679.83	Joback Method

Sources

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=C340045&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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