Benzeneethanol, 2,2,2-trifluoro-1-(3-chlorophenyl)

Inchi: InChI=1S/C8H6ClF3O/c9-6-3-1-2-5(4-6)7(13)8(10,11)12/h1-4,7,13H

InchiKey: IFUMGCOCVZUIRR-UHFFFAOYSA-N

Formula: C8H6ClF3O

SMILES: OC(c1cccc(Cl)c1)C(F)(F)F

Mol. weight [g/mol]: 210.58

Physical Properties

Property code	Value	Unit	Source
gf	-613.52	kJ/mol	Joback Method
hf	-753.72	kJ/mol	Joback Method
hfus	16.72	kJ/mol	Joback Method
hvap	53.27	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.936		Crippen Method
mcvol	123.240	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
rinpol	1206.00		NIST Webbook
rinpol	1206.00		NIST Webbook
tb	537.85	K	Joback Method
tc	728.45	K	Joback Method
tf	298.79	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.12	J/mol×K	537.85	Joback Method
cpg	285.30	J/mol×K	569.62	Joback Method
cpg	293.83	J/mol×K	601.38	Joback Method
cpg	301.75	J/mol×K	633.15	Joback Method
cpg	309.09	J/mol×K	664.92	Joback Method
cpg	315.88	J/mol×K	696.68	Joback Method
cpg	322.18	J/mol×K	728.45	Joback Method

Sources

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=R515172&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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