Benzeneethanol, 2,2-difluoro-1-(4-chlorophenyl)

Inchi: InChI=1S/C8H7ClF2O/c9-6-3-1-5(2-4-6)7(12)8(10)11/h1-4,7-8,12H

InchiKey: JGZVFDXSUANZDW-UHFFFAOYSA-N

Formula: C8H7ClF2O

SMILES: OC(c1ccc(Cl)cc1)C(F)F

Mol. weight [g/mol]: 192.59

Physical Properties

Property code	Value	Unit	Source
gf	-423.99	kJ/mol	Joback Method
hf	-554.14	kJ/mol	Joback Method
hfus	17.53	kJ/mol	Joback Method
hvap	54.99	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.639		Crippen Method
mcvol	121.470	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	1272.00		NIST Webbook
tb	541.37	K	Joback Method
tc	734.00	K	Joback Method
tf	280.78	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.41	J/mol×K	541.37	Joback Method
cpg	273.67	J/mol×K	573.47	Joback Method
cpg	282.38	J/mol×K	605.58	Joback Method
cpg	290.55	J/mol×K	637.68	Joback Method
cpg	298.21	J/mol×K	669.79	Joback Method
cpg	305.38	J/mol×K	701.89	Joback Method
cpg	312.08	J/mol×K	734.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515216&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