

Benzene, 1-chloro-4-(1-chloro-2,2-difluoroethyl)

Inchi:	InChI=1S/C8H6Cl2F2/c9-6-3-1-5(2-4-6)7(10)8(11)12/h1-4,7-8H
InchiKey:	YYIJGESQDVAVTP-UHFFFAOYSA-N
Formula:	C8H6Cl2F2
SMILES:	FC(F)C(Cl)c1ccc(Cl)cc1
Mol. weight [g/mol]:	211.04

Physical Properties

Property code	Value	Unit	Source
gf	-299.10	kJ/mol	Joback Method
hf	-417.65	kJ/mol	Joback Method
hfus	17.64	kJ/mol	Joback Method
hvap	42.70	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.885		Crippen Method
mcvol	127.840	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1218.00		NIST Webbook
tb	486.62	K	Joback Method
tc	697.45	K	Joback Method
tf	249.88	K	Joback Method
vc	0.497	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.91	J/mol×K	486.62	Joback Method
cpg	254.49	J/mol×K	521.76	Joback Method
cpg	264.38	J/mol×K	556.90	Joback Method
cpg	273.61	J/mol×K	592.04	Joback Method
cpg	282.21	J/mol×K	627.17	Joback Method
cpg	290.21	J/mol×K	662.31	Joback Method
cpg	297.64	J/mol×K	697.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515098&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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/45-720-2/Benzene-1-chloro-4-1-chloro-2-2-difluoroethyl.pdf>

Generated by Cheméo on 2024-04-28 02:02:44.508150637 +0000 UTC m=+16559013.428727949.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.