

Benzhydrol, 4,4'-dichloro-alpha-fluoromethyl-

Inchi:	InChI=1S/C14H11Cl2FO/c15-12-5-1-10(2-6-12)14(18,9-17)11-3-7-13(16)8-4-11/h1-8,18H
InchiKey:	RPYHUOWLWZFFZBP-UHFFFAOYSA-N
Formula:	C14H11Cl2FO
SMILES:	OC(CF)(c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	285.14
CAS:	116434-70-9

Physical Properties

Property code	Value	Unit	Source
gf	-80.09	kJ/mol	Joback Method
hf	-270.74	kJ/mol	Joback Method
hfus	27.47	kJ/mol	Joback Method
hvap	75.97	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.199		Crippen Method
mcvol	192.720	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
tb	746.12	K	Joback Method
tc	975.49	K	Joback Method
tf	449.09	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.02	J/molxK	746.12	Joback Method
cpg	494.95	J/molxK	784.35	Joback Method
cpg	504.98	J/molxK	822.58	Joback Method
cpg	514.19	J/molxK	860.80	Joback Method
cpg	522.67	J/molxK	899.03	Joback Method
cpg	530.51	J/molxK	937.26	Joback Method
cpg	537.80	J/molxK	975.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116434709&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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