

cis-Perfluorobicyclo[4.3.0]nonane

Inchi:

LnChI=1S/C9F16/c10-1-2(11,4(14,15)7(20,21)3(1,12)13)6(18,19)9(24,25)8(22,23)5(1,16)

InchiKey:

NLQOE OVORMKOIY-XIXRPRMCSA-N

Formula:

C9F16

SMILES:

FC1(F)C(F)(F)C(F)(F)C2(F)C(F)(F)C(F)(F)C(F)(F)C2(F)C1(F)F

Mol. weight [g/mol]:

412.07

CAS:

75262-87-2

Physical Properties

Property code	Value	Unit	Source
chl	-3151.40 ± 5.50	kJ/mol	NIST Webbook
gf	-3110.24	kJ/mol	Joback Method
hf	-3212.20 ± 5.60	kJ/mol	NIST Webbook
hfl	-3253.60 ± 5.60	kJ/mol	NIST Webbook
hfus	9.13	kJ/mol	Joback Method
hvap	41.40 ± 0.14	kJ/mol	NIST Webbook
log10ws	-5.51		Crippen Method
logp	4.877		Crippen Method
mcvol	144.270	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
tb	389.40	K	Joback Method
tc	522.36	K	Joback Method
tf	411.37	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.78	J/mol×K	500.20	Joback Method
cpg	372.94	J/mol×K	389.40	Joback Method
cpg	389.48	J/mol×K	411.56	Joback Method
cpg	404.05	J/mol×K	433.72	Joback Method
cpg	416.84	J/mol×K	455.88	Joback Method
cpg	428.02	J/mol×K	478.04	Joback Method
cpg	446.29	J/mol×K	522.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75262872&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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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