

2-endo,3-exo,5-endo,6-exo,8b,8c,10a,10c-octachloro

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C10H10Cl8/c1-9(7(15)16)2-3(11)5(13)10(9,8(17)18)6(14)4(2)12/h2-8H,1H3/t2

FCZHUROLVAKWCN-DHTDEGTBSA-N

C10H10Cl8

CC1(C(Cl)Cl)C2C(Cl)C(Cl)C1(C(Cl)Cl)C(Cl)C2Cl

413.81

Physical Properties

Property code	Value	Unit	Source
gf	-7.13	kJ/mol	Joback Method
hf	-317.99	kJ/mol	Joback Method
hfus	35.12	kJ/mol	Joback Method
hvap	68.31	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.660		Crippen Method
mcvol	227.960	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	2238.80		NIST Webbook
rinpol	2238.80		NIST Webbook
tb	721.64	K	Joback Method
tc	978.93	K	Joback Method
tf	470.78	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.01	J/mol×K	721.64	Joback Method
cpg	530.35	J/mol×K	764.52	Joback Method
cpg	543.58	J/mol×K	807.40	Joback Method
cpg	557.07	J/mol×K	850.29	Joback Method
cpg	571.20	J/mol×K	893.17	Joback Method
cpg	586.36	J/mol×K	936.05	Joback Method
cpg	602.92	J/mol×K	978.93	Joback Method

Sources

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=R502502&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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