Aldrin

Other names:

(1R,4S,4aS,5S,8R,8aR)-1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4:5,8-dimet
1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-Hexahydro-1,4-endo-exo-5,8-dimethanonaphthal
1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-1,4:5,8-dimethanonaphthalene, endo,exo-
1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-endo-1,4-exo-5,8-dimethanonaphthal
1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-endo-exo-1,4:5,8-dimethanonaphthale
1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-endo-exo-1,4:5,8-dimethylnaphthalen
1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-exo-1,4-endo-5,8-dimethanonaphthal
(aldrin)
1,2,3,4,10,10-Hexachloro-1«alpha»,4«alpha»,4a«beta»,5«alpha»,8«alpha»,8a«beta»-hex
1,2,3,4,10,10-Hexachloro-1Â«alphaÂ»,4Â«alphaÂ»,4aÂ«betaÂ»,5Â«alphaÂ»,8Â«alphaÂ
1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1«alpha»,4«alpha»,4a«beta»,5«alpha»,8«alpha»,8a«beta»)-
1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1Â«alphaÂ»,4Â«alphaÂ»,4aÂ«betaÂ»,5Â«alphaÂ»,8Â«alphaÂ»,8aÂ«betaÂ»)-
1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, endo,exo-
Aldocit
Aldrex
Aldrex 40
Aldrin Dust
Aldrin-R
Aldrine
Aldrite
Aldron
Aldrosol
Algran
Compound 118
Drinox
ENT 15,949
HHDN
HHPN
Hexachlorohexahydro-endo, exo-dimethanonaphthalene
Kortofin
NCI-C00044
OMS-194
Octalene
SD 2794
Seedrin
Tatuzinho
Tipula

Inchi: InChI=1S/C12H8Cl6/c13-8-9(14)11(16)7-5-2-1-4(3-5)6(7)10(8,15)12(11,17)18/h1-2,4-7H

InchiKey: QBYJBZPUGVGKQQ-SJJAEHHWSA-N

Formula: C12H8Cl6

SMILES: ClC1=C(Cl)C2(Cl)C3C4C=CC(C4)C3C1(Cl)C2(Cl)Cl

Mol. weight [g/mol]: 364.91
CAS: 309-00-2

Physical Properties

Property code	Value	Unit	Source
gf	222.64	kJ/mol	Joback Method
hf	-16.93	kJ/mol	Joback Method
hfus	30.54	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Joback Method
log10ws	-6.31		Estimated Solubility Method
logp	5.270		Crippen Method
mcvol	201.340	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1928.00		NIST Webbook
rinpol	1953.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	1948.72		NIST Webbook
rinpol	1928.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1943.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1953.00		NIST Webbook
rinpol	1987.00		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1928.00		NIST Webbook
rinpol	1929.00		NIST Webbook
rinpol	1933.00		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1943.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1933.00		NIST Webbook
rinpol	1932.18		NIST Webbook
rinpol	1939.62		NIST Webbook
rinpol	1948.72		NIST Webbook
rinpol	1946.47		NIST Webbook

rinpol	1950.51		NIST Webbook
rinpol	1959.90		NIST Webbook
rinpol	1961.08		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1943.00		NIST Webbook
rinpol	1946.00		NIST Webbook
rinpol	1950.00		NIST Webbook
ripol	2536.00		NIST Webbook
ripol	2537.00		NIST Webbook
ripol	2536.00		NIST Webbook
ripol	2502.00		NIST Webbook
ripol	2502.00		NIST Webbook
tb	720.49	K	Joback Method
tc	993.87	K	Joback Method
tf	377.00 ± 0.20	K	NIST Webbook
tf	372.00 ± 1.00	K	NIST Webbook
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.29	J/mol×K	948.30	Joback Method
cpg	473.55	J/mol×K	720.49	Joback Method
cpg	486.10	J/mol×K	766.05	Joback Method
cpg	499.48	J/mol×K	811.62	Joback Method
cpg	514.47	J/mol×K	857.18	Joback Method
cpg	531.81	J/mol×K	902.74	Joback Method
cpg	576.66	J/mol×K	993.87	Joback Method
hfust	4.15	kJ/mol	562.40	NIST Webbook
hsubt	91.80	kJ/mol	326.00	NIST Webbook
hvapt	75.10	kJ/mol	398.00	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.06740e+01
Coeff. B	-4.37206e+03
Coeff. C	-2.06700e+00
Temperature range (K), min.	423.01
Temperature range (K), max.	817.37

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C309002&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume