Dibenzo-p-dioxin, 1,2,3,6,7,9-hexachloro-

Inchi: InChI=1S/C12H2Cl6O2/c13-3-1-5(15)10-12(8(3)17)19-6-2-4(14)7(16)9(18)11(6)20-10/h1
InchiKey: BQOHWGKNRKCEFT-UHFFFAOYSA-N
Formula: C12H2Cl6O2
SMILES: Clc1cc2c(c(Cl)c1Cl)Oc1c(Cl)cc(Cl)c(Cl)c1O2
Mol. weight [g/mol]: 390.86
CAS: 64461-98-9

Physical Properties

Property code	Value	Unit	Source
gf	34.68	kJ/mol	Joback Method
hf	-168.85	kJ/mol	Joback Method
hfus	52.11	kJ/mol	Joback Method
hvap	87.53	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	7.505		Crippen Method
mcvol	206.740	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	2756.00		NIST Webbook
rinpol	2760.00		NIST Webbook
rinpol	2757.00		NIST Webbook
rinpol	2756.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	852.78	K	Joback Method
tc	1123.61	K	Joback Method
tf	636.36	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.83	J/mol×K	852.78	Joback Method
cpg	424.09	J/mol×K	897.92	Joback Method
cpg	429.98	J/mol×K	943.06	Joback Method
cpg	435.58	J/mol×K	988.19	Joback Method

cpg	440.99	J/mol×K	1033.33	Joback Method
cpg	446.32	J/mol×K	1078.47	Joback Method
cpg	451.65	J/mol×K	1123.61	Joback Method
dvisc	0.0009011	Pa×s	636.36	Joback Method
dvisc	0.0007551	Pa×s	672.43	Joback Method
dvisc	0.0006442	Pa×s	708.50	Joback Method
dvisc	0.0005581	Pa×s	744.57	Joback Method
dvisc	0.0004900	Pa×s	780.64	Joback Method
dvisc	0.0004352	Pa×s	816.71	Joback Method
dvisc	0.0003904	Pa×s	852.78	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64461989&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

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
rinpol: 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/113-359-8/Dibenzo-p-dioxin-1-2-3-6-7-9-hexachloro.pdf

Generated by Cheméo on 2025-12-21 09:37:22.440347104 +0000 UTC m=+6058039.970387768.

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