Bicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid, 1,4,5,6,7,7-hexachloro-, dibutyl ester

Other names: Chlorendic acid dibutyl ester
Dibutyl chlorendate
5-Norbornene-2,3-dicarboxylic acid, 1,4,5,6,7,7-hexachloro-, dibutyl ester
dibutyl 1,4,5,6,7,7-hexachlorobicyclo[2.2.1]hept-5-ene-2,3-dicarboxylate

Inchi: InChI=1S/C17H20Cl6O4/c1-3-5-7-26-13(24)9-10(14(25)27-8-6-4-2)16(21)12(19)11(18)15

InchiKey: UJAHPBDUQZFDLA-UHFFFAOYSA-N

Formula: C17H20Cl6O4

SMILES: CCCCOC(=O)C1C(C(=O)OCCCC)C2(Cl)C(Cl)=C(Cl)C1(Cl)C2(Cl)Cl

Mol. weight [g/mol]: 501.06

CAS: 1770-80-5

Physical Properties

Property code	Value	Unit	Source
gf	-366.66	kJ/mol	Joback Method
hf	-819.27	kJ/mol	Joback Method
hfus	49.48	kJ/mol	Joback Method
hvap	95.29	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.751		Crippen Method
mcvol	312.690	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
tb	979.10	K	Joback Method
tc	1214.37	K	Joback Method
tf	722.33	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.49	J/mol×K	979.10	Joback Method
cpg	939.11	J/mol×K	1018.31	Joback Method
cpg	967.08	J/mol×K	1057.52	Joback Method
cpg	997.79	J/mol×K	1096.74	Joback Method
cpg	1031.60	J/mol×K	1135.95	Joback Method

cpg	1068.91	J/mol×K	1175.16	Joback Method
cpg	1110.08	J/mol×K	1214.37	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=C1770805&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume