Dibutyl chlorendate

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

Physical Properties

Property code	Value	Unit	Source
af	0.7101		Cheméo Relay (1.0)
hf	-930.50	kJ/mol	Cheméo Relay (1.0)
hfus	49.48	kJ/mol	Joback Method
hvap	108.85	kJ/mol	Cheméo Relay (1.0)
ie	9.33	eV	Cheméo Relay (1.0)
log10ws	-6.85		Cheméo Relay (1.0)
logp	5.751		Crippen Method
mcvol	312.690	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
tb	633.22	K	Cheméo Relay (1.0)
tc	923.02	K	Cheméo Relay (1.0)
tf	348.94	K	Cheméo Relay (1.0)
vc	1.101	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1770805&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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