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

Other names: 5-Norbornene-2,3-dicarboxylic acid, 1,4,5,6,7,7-hexachloro-
Chlorendic acid
Hexachloroendomethylenetetrahydrophthalic acid
HET acid
Kyselina het
Kyselina 3,6-endomethylen-3,4,5,6,7,7-hexachlor-«delta»(4)-tetrahyroftalova
NCI-C55072
Kyselina 3,6-endomethylen-3,4,5,6,7,7-hexachlor-«delta»(4)-tetrahydroftalova
Kyselina 1,2,3,4,7,7-hexachlorbicyklo(2,2,1)hept-2-en-5,6-dikarboxylova
Bicyclo[2.2.1]-5-heptene-2,3-dicarboxylic acid, 1,4,5,6,7,7-hexachloro-
1,4,5,6,7,7-Hexachloro-5-norbornene-2,3-dicarboxylic acid
1,4,5,6,7,7-Hexachlorobicyclo-(2,2,1)hept-5-en-2,3-dicarboxylic acid
2H,3H-Hexachlorobicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid
NSC 22231
1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic acid

Inchi: InChI=1S/C9H4Cl6O4/c10-3-4(11)8(13)2(6(18)19)1(5(16)17)7(3,12)9(8,14)15/h1-2H,(H,1

InchiKey: DJKGDNKYTKCJKD-UHFFFAOYSA-N

Formula: C9H4Cl6O4

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

Mol. weight [g/mol]: 388.84

CAS: 115-28-6

Physical Properties

Property code	Value	Unit	Source
gf	-497.66	kJ/mol	Joback Method
hf	-694.17	kJ/mol	Joback Method
hfus	34.55	kJ/mol	Joback Method
hvap	106.02	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.234		Crippen Method
mcvol	199.970	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
tb	935.58	K	Joback Method
tc	1169.50	K	Joback Method
tf	709.35	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.24	J/mol×K	935.58	Joback Method
cpg	502.48	J/mol×K	974.57	Joback Method
cpg	521.39	J/mol×K	1013.55	Joback Method
cpg	543.36	J/mol×K	1052.54	Joback Method
cpg	568.77	J/mol×K	1091.53	Joback Method
cpg	598.00	J/mol×K	1130.51	Joback Method
cpg	631.45	J/mol×K	1169.50	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C115286&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

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