Bicyclo[2.2.2]-7-octene-2,3,5,6-tetracarboxylic acid dianhydride

Other names: 4,8-Etheno-1H,3H-benzo[1,2-c:4,5-c']difuran-1,3,5,7-tetrone, 3a,4,4a,7a,8,8a-hexahydro-bicyclo[2.2.2]oct-7-ene-2,3:5,6-tetracarboxylic dianhydride

Inchi: InChI=1S/C12H8O6/c13-9-5-3-1-2-4(7(5)11(15)17-9)8-6(3)10(14)18-12(8)16/h1-8H

InchiKey: XLOGCGOPKPCECW-UHFFFAOYSA-N

Formula: C12H8O6

SMILES: O=C1OC(=O)C2C3C=CC(C12)C1C(=O)OC(=O)C31

Mol. weight [g/mol]: 248.19

CAS: 1719-83-1

Physical Properties

Property code	Value	Unit	Source
gf	-379.10	kJ/mol	Joback Method
hf	-809.83	kJ/mol	Joback Method
hfus	32.54	kJ/mol	Joback Method
hvap	67.98	kJ/mol	Joback Method
log10ws	-0.10		Crippen Method
logp	-0.566		Crippen Method
mcvol	150.220	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	824.46	K	Joback Method
tc	1100.22	K	Joback Method
tf	608.02	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.40	J/mol×K	824.46	Joback Method
cpg	544.83	J/mol×K	870.42	Joback Method
cpg	558.45	J/mol×K	916.38	Joback Method
cpg	570.24	J/mol×K	962.34	Joback Method
cpg	580.16	J/mol×K	1008.30	Joback Method
cpg	588.19	J/mol×K	1054.26	Joback Method
cpg	594.29	J/mol×K	1100.22	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1719831&Units=SI
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
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