cis-Bicyclo[2.2.2]oct-5-en-2,3-dicarboxylic acid, anhydride

Other names: Bicyclo[2.2.2]oct-5-ene-2,3-dicarboxylic anhydride
Inchi: InChI=1S/C10H10O3/c11-9-7-5-1-2-6(4-3-5)8(7)10(12)13-9/h1-2,5-8H,3-4H2
InchiKey: YIHKILSPWGDWPR-UHFFFAOYSA-N
Formula: C10H10O3
SMILES: O=C1OC(=O)C2C3C=CC(CC3)C12
Mol. weight [g/mol]: 178.18
CAS: 6708-37-8

Physical Properties

Property code	Value	Unit	Source
gf	-117.68	kJ/mol	Joback Method
hf	-413.61	kJ/mol	Joback Method
hfus	21.15	kJ/mol	Joback Method
hvap	50.92	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	0.898		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	614.04	K	Joback Method
tc	867.97	K	Joback Method
tf	408.77	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.29	J/mol×K	614.04	Joback Method
cpg	371.76	J/mol×K	656.36	Joback Method
cpg	387.98	J/mol×K	698.68	Joback Method
cpg	403.01	J/mol×K	741.01	Joback Method
cpg	416.88	J/mol×K	783.33	Joback Method
cpg	429.62	J/mol×K	825.65	Joback Method
cpg	441.28	J/mol×K	867.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6708378&Units=SI

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

Latest version available from:
https://www.chemeo.com/cid/57-191-7/cis-Bicyclo-2-2-2-oct-5-en-2-3-dicarboxylic-acid-anhydride.pdf
Generated by Cheméo on 2024-10-12 04:32:01.304366238 +0000 UTC m=+3288383.941335490.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.