

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6708378&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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