

Carbic anhydride

Other names:

(3a«alpha»,4«alpha»,7«alpha»,7a«alpha»)-3a,4,7,7a-Tetrahydro-4,7-methano-isobenzofuran-1,3-dione, 3a,4,7,7a-tetrahydro-,
4,7-Methanoisobenzofuran-1,3-dione, 3a,4,7,7a-tetrahydro-,
(3a«alpha»,4«alpha»,7«alpha»,7a«alpha»)-
8,9,10-Trihydro-5-ene-2,3-dicarboxylic anhydride
endo-Himic acid anhydride
endo-3,6-Methylene-1,2,3,6-tetrahydrophthalic anhydride
endo-5-Norbornene-2,3-dicarboxylic anhydride
endo,cis-5-Norbornene-2,3-dicarboxylic anhydride
Endic anhydride
Nadic anhydride
3,6-Endomethylene-«delta»4-tetrahydrophthalic anhydride
5-Norbornene-endo-2,3-dicarboxylic anhydride
5-Norbornene-2,3-dicarboxylic anhydride, cis-endo-
4,7-Methanoisobenzofuran-1,3-dione, 3a,4,7,7a-tetrahydro-, (3aR,4S,7R,7aS)-rel-
Bicyclo[2.2.1]hept-5-ene-2-endo,3-endo-dicarboxylic anhydride
Bicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid endo-cis-anhydride
cis-5-Norbornene-endo-2,3-dicarboxylic anhydride
NSC 102277

Inchi:

InChI=1S/C9H8O3/c10-8-6-4-1-2-5(3-4)7(6)9(11)12-8/h1-2,4-7H,3H2/t4-,5-,6-,7+/m0/s1

InchiKey:

KNDQHSIWLOJIGP-ZTYPAAOSTSA-N

Formula:

C9H8O3

SMILES:

O=C1OC(=O)C2C3C=CC(C3)C12

Mol. weight [g/mol]:

164.16

CAS:

129-64-6

Physical Properties

Property code	Value	Unit	Source
gf	-114.00	kJ/mol	Joback Method
hf	-386.81	kJ/mol	Joback Method
hfus	20.66	kJ/mol	Joback Method
hsub	97.00 ± 4.20	kJ/mol	NIST Webbook
hvap	48.53	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.508		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	586.89	K	Joback Method
tc	837.54	K	Joback Method

tf	401.02	K	Joback Method
tt	435.40 ± 1.00	K	NIST Webbook
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.71	J/mol×K	586.89	Joback Method
cpg	320.44	J/mol×K	628.67	Joback Method
cpg	335.09	J/mol×K	670.44	Joback Method
cpg	348.69	J/mol×K	712.22	Joback Method
cpg	361.29	J/mol×K	753.99	Joback Method
cpg	372.95	J/mol×K	795.77	Joback Method
cpg	383.70	J/mol×K	837.54	Joback Method
hfust	3.71	kJ/mol	437.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C129646&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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
tt:	Triple Point Temperature
vc:	Critical Volume

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