3-Methyl-4-cyclohexene-1,2-dicarboxylic anhydride

Other names: 1,3-Isobenzofurandione, 3a,4,7,7a-tetrahydro-4-methyl-
Maleic anhydride and 1,3-pentadiene adduct
1,2,3,6-Tetrahydro-3-methylphthalic anhydride
3-Methyl-«delta»4-tetrahydrophthalic anhydride
3-Methyl-1,2,3,6-tetrahydrophthalic anhydride
3-Methyltetrahydrophthalic anhydride
4-Cyclohexene-1,2-dicarboxylic anhydride, 3-methyl-
NSC 2352

Inchi: InChI=1S/C9H10O3/c1-5-3-2-4-6-7(5)9(11)12-8(6)10/h2-3,5-7H,4H2,1H3

InchiKey: XPEKVUUBSDFMDR-UHFFFAOYSA-N

Formula: C9H10O3

SMILES: CC1C=CCC2C(=O)OC(=O)C12

Mol. weight [g/mol]: 166.17

CAS: 5333-84-6

Physical Properties

Property code	Value	Unit	Source
gf	-198.95	kJ/mol	Joback Method
hf	-471.93	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	48.96	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	0.898		Crippen Method
mcvol	120.660	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	588.69	K	Joback Method
tc	838.56	K	Joback Method
tf	376.04	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.30	J/mol×K	588.69	Joback Method

cpg	338.36	J/mol×K	630.34	Joback Method
cpg	354.38	J/mol×K	671.98	Joback Method
cpg	369.33	J/mol×K	713.63	Joback Method
cpg	383.21	J/mol×K	755.27	Joback Method
cpg	395.97	J/mol×K	796.92	Joback Method
cpg	407.61	J/mol×K	838.56	Joback Method

Sources

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=C5333846&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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