

1,3-Isobenzofurandione, 3a,4,7,7a-tetrahydro-5-methyl-

Other names:	Isomethyltetrahydrophthalic anhydride 4-Cyclohexene-1,2-dicarboxylic anhydride, 4-methyl- 4-Methyl-«delta»-4-tetrahydrophthalic anhydride 4-Methyl-1,2,3,6-tetrahydrophthalic anhydride 4-Methyltetrahydrophthalic anhydride 4-Methyl-cyclohex-4-en-1,2-dicarboxylic acid anhydride 5-Methyl-3a,4,7,7a-tetrahydro-2-benzofuran-1,3-dione 1,2,3,6-Tetrahydro-4-methylphthalic anhydride NSC 52669 4-Methyl-4-cyclohexene-1,2-dicarboxylic anhydride
Inchi:	InChI=1S/C9H10O3/c1-5-2-3-6-7(4-5)9(11)12-8(6)10/h2,6-7H,3-4H2,1H3
InchiKey:	OEMSKMUAMXLNKL-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	CC1=CCC2C(=O)OC(=O)C2C1
Mol. weight [g/mol]:	166.17
CAS:	3425-89-6

Physical Properties

Property code	Value	Unit	Source
gf	-200.87	kJ/mol	Joback Method
hf	-463.06	kJ/mol	Joback Method
hfus	16.87	kJ/mol	Joback Method
hvap	49.93	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.042		Crippen Method
mcvol	120.660	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	598.34	K	Joback Method
tc	849.13	K	Joback Method
tf	392.80	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.84	J/mol×K	598.34	Joback Method
cpg	335.09	J/mol×K	640.14	Joback Method
cpg	350.36	J/mol×K	681.94	Joback Method
cpg	364.62	J/mol×K	723.74	Joback Method
cpg	377.85	J/mol×K	765.54	Joback Method
cpg	390.03	J/mol×K	807.33	Joback Method
cpg	401.13	J/mol×K	849.13	Joback Method
hfust	17.67	kJ/mol	220.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3425896&Units=SI
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

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
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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