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

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]: 166.18

Physical Properties

Property code	Value	Unit	Source
hfus	16.87	kJ/mol	Joback Method
logp	1.042		Crippen Method
mcvol	120.660	ml/mol	McGowan Method
tb	556.57	K	Cheméo Relay (1.0)

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3425896&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature