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

Other names:	4-Cyclohexene-1,2-dicarboxylic anhydride
	«DELTA»4-Tetrahydrophthalic anhydride
	Butadiene-maleic anhydride adduct
	Maleic anhydride adduct of butadiene
	Tetrahydrophthalic acid anhydride
	Tetrahydrophthalic anhydride
	1,2,3,6-Tetrahydrophthalic acid anhydride
	1,2,3,6-Tetrahydrophthalic anhydride
	4-Cyclohexene-1,2-dicarboxylic acid anhydride
	Anhydrid kyseliny tetrahydroftalove
	Memtetrahydro phtalic anhydride
	Phthalic anhydride, 1,2,3,6-tetrahydro-
	Tetrahydroftalanhydrid
	THPA
	Cyclohex-4-en-1,2-dicarboxylic acid anhydride
	NSC 82642
	Rikacid TH
Inchi:	InChI=1S/C8H8O3/c9-7-5-3-1-2-4-6(5)8(10)11-7/h1-2,5-6H,3-4H2
InchiKey:	KMOUUZVZFBCRAM-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	O=C1OC(=O)C2CC=CCC12
Mol. weight [g/mol]:	152.15
CAS:	85-43-8

Physical Properties

Property code	Value	Unit	Source
gf	-199.66	kJ/mol	Joback Method
hf	-430.95	kJ/mol	Joback Method
hfus	14.67	kJ/mol	Joback Method
hvap	47.04	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.652		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
tb	570.48	K	Joback Method
tc	825.93	K	Joback Method
tf	369.01	K	Joback Method

vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.11	J/mol×K	570.48	Joback Method
cpg	287.75	J/mol×K	613.06	Joback Method
cpg	302.42	J/mol×K	655.63	Joback Method
cpg	316.11	J/mol×K	698.21	Joback Method
cpg	328.79	J/mol×K	740.78	Joback Method
cpg	340.45	J/mol×K	783.36	Joback Method
cpg	351.08	J/mol×K	825.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85438&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

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