1,3-Isobenzofurandione, hexahydro-, trans-

Other names: trans-Cyclohexane-1,2-dicarboxylic anhydride
Hexahydro-2-benzofuran-1,3-dione, trans
Inchi: InChI=1S/C8H10O3/c9-7-5-3-1-2-4-6(5)8(10)11-7/h5-6H,1-4H2/t5-,6-/m0/s1
InchiKey: MUTGBJKUEZFXGO-WDSKDSINSA-N
Formula: C8H10O3
SMILES: O=C1OC(=O)C2CCCCC12
Mol. weight [g/mol]: 154.16
CAS: 14166-21-3

Physical Properties

Property code	Value	Unit	Source
chs	-3919.60 ± 0.20	kJ/mol	NIST Webbook
gf	-229.62	kJ/mol	Joback Method
hf	-488.73	kJ/mol	Joback Method
hfus	13.44	kJ/mol	Joback Method
hvap	46.75	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	0.876		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	571.32	K	Joback Method
tc	824.11	K	Joback Method
tf	368.25	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.71	J/mol×K	571.32	Joback Method
cpg	308.71	J/mol×K	613.45	Joback Method
cpg	324.69	J/mol×K	655.58	Joback Method
cpg	339.63	J/mol×K	697.72	Joback Method
cpg	353.51	J/mol×K	739.85	Joback Method
cpg	366.32	J/mol×K	781.98	Joback Method

cpg	378.03	J/mol×K	824.11	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=C14166213&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
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