Homophthalic anhydride

Other names:	1H-2-Benzopyran-1,3(4H)-dione
	1,3-Isochromandione
	3,4-2H-Isocoumarin-3-one
	benzoglutaric anhydride
Inchi:	InChI=1S/C9H6O3/c10-8-5-6-3-1-2-4-7(6)9(11)12-8/h1-4H,5H2
InchiKey:	AKHSBAVQPIRVAG-UHFFFAOYSA-N
Formula:	C9H6O3
SMILES:	O=C1Cc2ccccc2C(=O)O1
Mol. weight [g/mol]:	162.14
CAS:	703-59-3

Physical Properties

Property code	Value	Unit	Source
gf	-147.26	kJ/mol	Joback Method
hf	-324.45	kJ/mol	Joback Method
hfus	14.68	kJ/mol	Joback Method
hvap	51.96	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	0.926		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
tb	615.25	K	Joback Method
tc	881.29	K	Joback Method
tf	411.80	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.52	J/mol×K	615.25	Joback Method
cpg	285.76	J/mol×K	659.59	Joback Method
cpg	298.07	J/mol×K	703.93	Joback Method
cpg	309.42	J/mol×K	748.27	Joback Method
cpg	319.79	J/mol×K	792.61	Joback Method

cpg	329.17	J/mol×K	836.95	Joback Method
cpg	337.53	J/mol×K	881.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C703593&Units=SI

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