

2,3-Benzofurandione

Other names:	Coumarandione
Inchi:	InChI=1S/C8H4O3/c9-7-5-3-1-2-4-6(5)11-8(7)10/h1-4H
InchiKey:	UUISWLJHAJBRAA-UHFFFAOYSA-N
Formula:	C8H4O3
SMILES:	O=C1Oc2ccccc2C1=O
Mol. weight [g/mol]:	148.12
CAS:	4732-72-3

Physical Properties

Property code	Value	Unit	Source
gf	-143.58	kJ/mol	Joback Method
hf	-297.65	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	49.57	kJ/mol	Joback Method
ie	9.65 ± 0.05	eV	NIST Webbook
log10ws	-1.50		Crippen Method
logp	0.788		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	588.10	K	Joback Method
tc	850.92	K	Joback Method
tf	407.00	K	NIST Webbook
vc	0.368	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.20	J/mol×K	588.10	Joback Method
cpg	237.41	J/mol×K	631.90	Joback Method
cpg	247.88	J/mol×K	675.71	Joback Method
cpg	257.60	J/mol×K	719.51	Joback Method
cpg	266.56	J/mol×K	763.31	Joback Method
cpg	274.75	J/mol×K	807.11	Joback Method
cpg	282.16	J/mol×K	850.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.20	K	2.30	NIST Webbook
tbrp	415.00	K	2.30	NIST Webbook

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=C4732723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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