1,2,4-BENZENETRICARBOXYLIC 1,2-ANHYDRIDE

Other names: 1,2,4-BENZENETRICARBOXYLIC ACID
1,2,4-Benzenetricarboxylic acid 1,2-anhydride
1,2,4-Benzenetricarboxylic acid anhydride
1,2,4-Benzenetricarboxylic acid anhydride-1,2
1,2,4-Benzenetricarboxylic acid, cyclic 1,2-anhydride
1,2,4-Benzenetricarboxylic anhydride
1,3-Dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid
1,3-Dioxo-5-phthalancarboxylic acid
4-Carboxyphthalic anhydride
5-Isobenzofurancarboxylic acid, 1,3-dihydro-1,3-dioxo-
5-Phthalanacarboxylic acid, 1,3-dioxo-
Anhydrotrimellic acid
Anhydrotrimellitic acid
Benzene-1,2,4-tricarboxylic-1,2-anhydride
Epon 9150
NCI-C56633
NSC 60252
TMA
TMAN
TRIMELLITIC ACID ANHYDRIDE
TRIMELLITIC ANHYDRIDE
Trimellic acid anhydride
Trimellic acid-1,2-anhydride
Trimellitic acid 1,2-anhydride
Trimellitic acid cyclic 1,2-anhydride
benzene-1,2,4-tricarboxylic acid 1,2-anhydride

Inchi: InChI=1S/C9H4O5/c10-7(11)4-1-2-5-6(3-4)9(13)14-8(5)12/h1-3H,(H,10,11)

InchiKey: SRPWOOOHEPICQU-UHFFFAOYSA-N

Formula: C9H4O5

SMILES: O=C(O)c1ccc2c(c1)C(=O)OC2=O

Mol. weight [g/mol]: 192.13

CAS: 552-30-7

Physical Properties

Property code	Value	Unit	Source
af	0.8300		Cheméo Relay (1.0)

gf	-410.53	kJ/mol	Joback Method
hf	-764.28	kJ/mol	Cheméo Relay (1.0)
hfus	22.08	kJ/mol	Joback Method
hvap	99.72	kJ/mol	Cheméo Relay (1.0)
ie	10.78	eV	Cheméo Relay (1.0)
log10ws	-2.36		Cheméo Relay (1.0)
logp	0.695		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
tb	607.46	K	Cheméo Relay (1.0)
tc	914.82	K	Cheméo Relay (1.0)
tf	385.00 ± 2.00	K	NIST Webbook
tf	385.00 ± 2.00	K	NIST Webbook
vc	0.456	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.86	J/mol×K	881.69	Joback Method
cpg	347.93	J/mol×K	921.58	Joback Method
cpg	327.43	J/mol×K	801.90	Joback Method
cpg	353.23	J/mol×K	961.48	Joback Method
cpg	319.10	J/mol×K	762.01	Joback Method
cpg	357.73	J/mol×K	1001.37	Joback Method
cpg	335.02	J/mol×K	841.80	Joback Method
cps	248.90	J/mol×K	298.15	NIST Webbook
hfust	10.46	kJ/mol	385.00	NIST Webbook
hfust	10.46	kJ/mol	385.00	NIST Webbook
hfust	10.46	kJ/mol	385.00	NIST Webbook
hvapt	65.60	kJ/mol	577.00	NIST Webbook
sfust	27.20	J/mol×K	385.00	NIST Webbook
sfust	27.20	J/mol×K	385.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=994

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C552307&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume