Benzo[rst]pentaphene-5,8-dione

Inchi: InChI=1S/C24H14O2/c25-23-17-7-3-1-5-13(17)15-9-10-16-14-6-2-4-8-18(14)24(26)20-12
InchiKey: FMVVSOMDKCGKDW-UHFFFAOYSA-N
Formula: C24H12O2
SMILES: O=C1c2ccccc2-c2ccc3c4c(ccc1c24)C(=O)C1C=CC=CC31
Mol. weight [g/mol]: 332.35
CAS: 3302-52-1

Physical Properties

Property code	Value	Unit	Source
chs	-10908.10 ± 6.70	kJ/mol	NIST Webbook
gf	451.32	kJ/mol	Joback Method
hf	153.15	kJ/mol	Joback Method
hfus	37.97	kJ/mol	Joback Method
hsub	113.00	kJ/mol	NIST Webbook
hvap	87.47	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	5.073		Crippen Method
mcvol	244.000	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
tb	1000.34	K	Joback Method
tc	1280.40	K	Joback Method
tf	707.92	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.02	J/mol×K	1000.34	Joback Method
cpg	796.50	J/mol×K	1047.02	Joback Method
cpg	811.64	J/mol×K	1093.69	Joback Method
cpg	826.72	J/mol×K	1140.37	Joback Method
cpg	842.00	J/mol×K	1187.04	Joback Method
cpg	857.71	J/mol×K	1233.72	Joback Method
cpg	874.13	J/mol×K	1280.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3302521&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hsub:	Enthalpy of sublimation 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