9,10-Anthracenedione, 2-(1,1-dimethylethyl)-

Other names:	2-(tert-butyl)anthracene-9,10-dione
	2-tert-Butyl-9,10-anthraquinone
	2-tert-butylanthraquinone
	Anthraquinone, 2-tert-butyl-
	«beta»-tert-Butylanthraquinone
Inchi:	InChI=1S/C18H16O2/c1-18(2,3)11-8-9-14-15(10-11)17(20)13-7-5-4-6-12(13)16(14)19/h4
InchiKey:	YTPSFXZMJKMUJE-UHFFFAOYSA-N
Formula:	C18H16O2
SMILES:	CC(C)(C)c1ccc2c(c1)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]:	264.32
CAS:	84-47-9

Physical Properties

Property code	Value	Unit	Source
ea	1.56 ± 0.06	eV	NIST Webbook
gf	134.83	kJ/mol	Joback Method
hf	-161.05	kJ/mol	Joback Method
hfus	20.06	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.760		Crippen Method
mcvol	209.240	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
tb	819.09	K	Joback Method
tc	1084.31	K	Joback Method
tf	547.58	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.68	J/mol×K	1040.11	Joback Method
cpg	616.33	J/mol×K	819.09	Joback Method
cpg	632.14	J/mol×K	863.29	Joback Method

cpg	646.59	J/mol×K	907.50	Joback Method
cpg	659.76	J/mol×K	951.70	Joback Method
cpg	671.76	J/mol×K	995.90	Joback Method
cpg	692.61	J/mol×K	1084.31	Joback Method
hvapt	101.40	kJ/mol	503.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of 2-Ethylanthraquinone in Binary Mixtures of Oligooxymethylene Dimethyl Ethers with Different Number of CH2O Groups of n = 2, 3, and 4 from 293.15 to 343.15 K:	https://www.doi.org/10.1021/acs.jced.6b00334
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=C84479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
hvapt:	Enthalpy of vaporization at a given temperature
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