9,10-Anthracenedione, 2-ethyl-

Other names:	2-Ethyl-9,10-anthraquinone
	2-ethyl-9,10-anthracenedione
	2-ethylanthraquinone
	Anthraquinone, 2-ethyl-
	USAF so-1
Inchi:	InChI=1S/C16H12O2/c1-2-10-7-8-13-14(9-10)16(18)12-6-4-3-5-11(12)15(13)17/h3-9H,2H
InchiKey:	SJEBAWHUJDUKQK-UHFFFAOYSA-N
Formula:	C16H12O2
SMILES:	CCc1ccc2c(c1)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]:	236.27
CAS:	84-51-5

Physical Properties

Property code	Value	Unit	Source
ea	1.56 ± 0.06	eV	NIST Webbook
gf	115.15	kJ/mol	Joback Method
hf	-111.02	kJ/mol	Joback Method
hfus	18.79	kJ/mol	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
hvap	66.29	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.024		Crippen Method
mcvol	181.060	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2122.00		NIST Webbook
tb	776.56	K	Joback Method
tc	1039.27	K	Joback Method
tf	522.62	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.16	J/mol×K	776.56	Joback Method
cpg	519.99	J/mol×K	820.35	Joback Method
cpg	533.57	J/mol×K	864.13	Joback Method
cpg	545.93	J/mol×K	907.92	Joback Method
cpg	557.13	J/mol×K	951.70	Joback Method
cpg	567.20	J/mol×K	995.49	Joback Method
cpg	576.18	J/mol×K	1039.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84515&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume