

Anthracene-maleic anhydride Diels-Alder adduct

Other names:

Anthracene, 2,5-furandione adduct
Anthracene,maleic anhydride adduct
endo-9,10-(«alpha», «beta»-Succinic anhydride)anthracene
9,10(3',4')-Furanoanthracene-12,14-dione
9,10-Dihydroanthraceno-9,10-endo-«alpha», «beta»-succinic anhydride
9,10-Ethanoanthracene-11,12-dicarboxylic anhydride

Inchi: InChI=1S/C18H12O3/c19-17-15-13-9-5-1-2-6-10(9)14(16(15)18(20)21-17)12-8-4-3-7-11

InchiKey: PSKVQQJLLWSBFV-UHFFFAOYSA-N

Formula: C18H12O3

SMILES: O=C1OC(=O)C2C3c4cccc4C(c4cccc43)C12

Mol. weight [g/mol]: 276.29

CAS: 5443-16-3

Physical Properties

Property code	Value	Unit	Source
chs	-8380.00 ± 5.90	kJ/mol	NIST Webbook
gf	173.68	kJ/mol	Joback Method
hf	-161.75	kJ/mol	Joback Method
hfs	-418.20 ± 6.40	kJ/mol	NIST Webbook
hfus	36.35	kJ/mol	Joback Method
hvap	73.63	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.593		Crippen Method
mcvol	193.390	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
tb	844.16	K	Joback Method
tc	1114.96	K	Joback Method
tf	590.13	K	Joback Method
vc	0.749	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.70	J/mol×K	844.16	Joback Method

cpg	631.27	J/mol×K	889.29	Joback Method
cpg	645.69	J/mol×K	934.43	Joback Method
cpg	659.12	J/mol×K	979.56	Joback Method
cpg	671.74	J/mol×K	1024.69	Joback Method
cpg	683.70	J/mol×K	1069.82	Joback Method
cpg	695.17	J/mol×K	1114.96	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=C5443163&Units=SI

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
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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