

Anthracene photodimer

Other names:	Anthracene, dimer Dianthracene 5,12:6,11-Di-o-benzenodibenzo(a,e)cyclooctene, 5,6,11,12-tetrahydro- 5,12(1',2'):6,11(1'',2'')-Dibenzenodibenzo(a,e)cyclooctene, 5,6,11,12-tetrahydro-
Inchi:	InChI=1S/C28H20/c1-2-10-18-17(9-1)25-19-11-3-4-12-20(19)26(18)28-23-15-7-5-13-21(12)
InchiKey:	JUTIJVADGQDBGY-UHFFFAOYSA-N
Formula:	C28H20
SMILES:	<chem>c1ccc2c(c1)C1c3ccccc3C2C2c3ccccc3C1c1cccc12</chem>
Mol. weight [g/mol]:	356.46
CAS:	1627-06-1

Physical Properties

Property code	Value	Unit	Source
chs	-14169.00	kJ/mol	NIST Webbook
chs	-14183.00	kJ/mol	NIST Webbook
gf	831.04	kJ/mol	Joback Method
hf	507.85	kJ/mol	Joback Method
hfs	306.00	kJ/mol	NIST Webbook
hfus	48.86	kJ/mol	Joback Method
hvap	88.24	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	6.555		Crippen Method
mcvol	277.760	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
tb	960.88	K	Joback Method
tc	1229.65	K	Joback Method
tf	628.26	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.83	J/molxK	960.88	Joback Method
cpg	917.02	J/molxK	1005.68	Joback Method

cpg	936.42	J/molxK	1050.47	Joback Method
cpg	956.42	J/molxK	1095.27	Joback Method
cpg	977.42	J/molxK	1140.06	Joback Method
cpg	999.82	J/molxK	1184.86	Joback Method
cpg	1024.03	J/molxK	1229.65	Joback Method
dvisc	0.0144615	Paxs	628.26	Joback Method
dvisc	0.0144363	Paxs	683.70	Joback Method
dvisc	0.0144149	Paxs	739.13	Joback Method
dvisc	0.0143966	Paxs	794.57	Joback Method
dvisc	0.0143806	Paxs	850.01	Joback Method
dvisc	0.0143667	Paxs	905.44	Joback Method
dvisc	0.0143543	Paxs	960.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1627061&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mccvol:	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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