

9,9'-Bianthracene

Other names:	9,9'-Bianthracenyl 9,9'-Bianthranyl 9,9'-Bianthryl 9,9'-Dianthracene 9-(9-Anthryl)anthracene
Inchi:	InChI=1S/C28H18/c1-5-13-23-19(9-1)17-20-10-2-6-14-24(20)27(23)28-25-15-7-3-11-21(2)
InchiKey:	SXGIRTCIFPJUEQ-UHFFFAOYSA-N
Formula:	C28H18
SMILES:	<chem>c1ccc2c(-c3c4ccccc4cc4ccccc34)c3ccccc3cc2c1</chem>
Mol. weight [g/mol]:	354.44
CAS:	1055-23-8

Physical Properties

Property code	Value	Unit	Source
chs	-13917.60 ± 3.10	kJ/mol	NIST Webbook
gf	797.78	kJ/mol	Joback Method
hf	475.00	kJ/mol	NIST Webbook
hfs	326.90 ± 4.80	kJ/mol	NIST Webbook
hfus	42.88	kJ/mol	Joback Method
hsub	148.00	kJ/mol	NIST Webbook
hvap	91.68	kJ/mol	Joback Method
log10ws	-11.29		Crippen Method
logp	7.966		Crippen Method
mcvol	280.020	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
tb	989.24	K	Joback Method
tc	1268.29	K	Joback Method
tf	639.04	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.81	J/mol×K	1221.78	Joback Method

cpg	899.10	J/molxK	1128.76	Joback Method
cpg	881.61	J/molxK	1082.26	Joback Method
cpg	864.57	J/molxK	1035.75	Joback Method
cpg	847.59	J/molxK	989.24	Joback Method
cpg	917.37	J/molxK	1175.27	Joback Method
cpg	957.76	J/molxK	1268.29	Joback Method
dvisc	0.0018094	Paxs	639.04	Joback Method
dvisc	0.0007382	Paxs	989.24	Joback Method
dvisc	0.0008179	Paxs	930.87	Joback Method
dvisc	0.0009188	Paxs	872.51	Joback Method
dvisc	0.0010495	Paxs	814.14	Joback Method
dvisc	0.0012236	Paxs	755.77	Joback Method
dvisc	0.0014638	Paxs	697.41	Joback Method
hsubt	148.00	kJ/mol	293.00	NIST Webbook
hsubt	127.90	kJ/mol	443.00	NIST Webbook
hsubt	128.00 ± 4.20	kJ/mol	413.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	5.52364e+01
Coeff. B	-3.52203e+04
Temperature range (K), min.	640.97
Temperature range (K), max.	705.47

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1055238&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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