

Anthra[9,1,2-abc]coronene

Inchi:

InChI=1S/C34H16/c1-2-4-24-20(3-1)15-21-11-12-23-16-22-10-9-18-6-5-17-7-8-19-13-14

InchiKey:

GOQXCYPJSAHUAZ-UHFFFAOYSA-N

Formula:

C34H16

SMILES:

c1ccc2c(c1)cc1ccc3cc4ccc5ccc6ccc7ccc8c2c1c3c1c4c5c6c7c81

Mol. weight [g/mol]:

424.49

CAS:

128345-73-3

Physical Properties

Property code	Value	Unit	Source
gf	1207.58	kJ/mol	Joback Method
hf	937.47	kJ/mol	Joback Method
hfus	59.83	kJ/mol	Joback Method
hvap	111.07	kJ/mol	Joback Method
log10ws	-15.37		Crippen Method
logp	9.817		Crippen Method
mcvol	308.220	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
tb	1183.86	K	Joback Method
tc	1465.19	K	Joback Method
tf	918.94	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.98	J/mol×K	1183.86	Joback Method
cpg	1086.84	J/mol×K	1230.75	Joback Method
cpg	1134.65	J/mol×K	1277.64	Joback Method
cpg	1189.14	J/mol×K	1324.53	Joback Method
cpg	1251.03	J/mol×K	1371.42	Joback Method
cpg	1321.06	J/mol×K	1418.30	Joback Method
cpg	1399.93	J/mol×K	1465.19	Joback Method
dvisc	0.4024121	Pa×s	918.94	Joback Method
dvisc	0.4201945	Pa×s	963.09	Joback Method

dvisc	0.4371025	Pa×s	1007.25	Joback Method
dvisc	0.4531868	Pa×s	1051.40	Joback Method
dvisc	0.4684964	Pa×s	1095.55	Joback Method
dvisc	0.4830780	Pa×s	1139.71	Joback Method
dvisc	0.4969759	Pa×s	1183.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C128345733&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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