

Naphtho[8,1,2-abc]coronene

Inchi:	InChI=1S/C30H14/c1-2-15-8-10-19-14-20-11-9-17-5-4-16-6-7-18-12-13-22-21(3-1)23(15)
InchiKey:	NWMLYQXCXBWZRG-UHFFFAOYSA-N
Formula:	C30H14
SMILES:	<chem>c1cc2ccc3cc4ccc5ccc6ccc7ccc8c(c1)c2c3c1c4c5c6c7c81</chem>
Mol. weight [g/mol]:	374.43
CAS:	6596-38-9

Physical Properties

Property code	Value	Unit	Source
gf	1076.88	kJ/mol	Joback Method
hf	840.43	kJ/mol	Joback Method
hfus	52.84	kJ/mol	Joback Method
hvap	99.86	kJ/mol	Joback Method
log10ws	-13.57		Crippen Method
logp	8.663		Crippen Method
mcvol	271.320	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
tb	1068.38	K	Joback Method
tc	1339.64	K	Joback Method
tf	828.64	K	Joback Method
vc	1.103	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.33	J/molxK	1068.38	Joback Method
cpg	872.72	J/molxK	1113.59	Joback Method
cpg	902.72	J/molxK	1158.80	Joback Method
cpg	936.92	J/molxK	1204.01	Joback Method
cpg	975.91	J/molxK	1249.22	Joback Method
cpg	1020.28	J/molxK	1294.43	Joback Method
cpg	1070.64	J/molxK	1339.64	Joback Method
dvisc	0.2034947	Paxs	828.64	Joback Method
dvisc	0.2138556	Paxs	868.60	Joback Method

dvisc	0.2237645	Paxs	908.55	Joback Method
dvisc	0.2332407	Paxs	948.51	Joback Method
dvisc	0.2423043	Paxs	988.47	Joback Method
dvisc	0.2509756	Paxs	1028.42	Joback Method
dvisc	0.2592744	Paxs	1068.38	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=C6596389&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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