

Benzo[a]coronene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C28H14/c1-2-4-20-19(3-1)21-13-11-17-9-7-15-5-6-16-8-10-18-12-14-22(20)28

NQSLOOOUQZYGEB-UHFFFAOYSA-N

C28H14

c1ccc2c(c1)c1ccc3ccc4ccc5ccc6ccc2c2c6c5c4c3c12

350.41

190-70-5

Physical Properties

Property code	Value	Unit	Source
gf	968.78	kJ/mol	Joback Method
hf	747.57	kJ/mol	Joback Method
hfus	48.05	kJ/mol	Joback Method
hvap	93.74	kJ/mol	Joback Method
ie	7.08	eV	NIST Webbook
ie	7.08	eV	NIST Webbook
ie	7.08	eV	NIST Webbook
log10ws	-12.35		Crippen Method
logp	8.072		Crippen Method
mcvol	258.300	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	656.34		NIST Webbook
rinpol	655.84		NIST Webbook
rinpol	655.84		NIST Webbook
tb	1006.36	K	Joback Method
tc	1275.89	K	Joback Method
tf	754.60	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.55	J/mol×K	1006.36	Joback Method
cpg	797.63	J/mol×K	1051.28	Joback Method
cpg	819.89	J/mol×K	1096.20	Joback Method

cpg	844.84	J/mol×K	1141.13	Joback Method
cpg	872.97	J/mol×K	1186.05	Joback Method
cpg	904.81	J/mol×K	1230.97	Joback Method
cpg	940.85	J/mol×K	1275.89	Joback Method
dvisc	0.0530229	Pa×s	754.60	Joback Method
dvisc	0.0545360	Pa×s	796.56	Joback Method
dvisc	0.0559346	Pa×s	838.52	Joback Method
dvisc	0.0572308	Pa×s	880.48	Joback Method
dvisc	0.0584351	Pa×s	922.44	Joback Method
dvisc	0.0595567	Pa×s	964.40	Joback Method
dvisc	0.0606036	Pa×s	1006.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C190705&Units=SI
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

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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