BENZO[A]CORONENE

Inchi: 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-
InchiKey: NQSLOOOUQZYGEB-UHFFFAOYSA-N
Formula: C28H14
SMILES: c1ccc2c(c1)c1ccc3ccc4ccc5ccc6ccc2c2c6c5c4c3c12
Mol. weight [g/mol]: 350.42

Physical Properties

Property code	Value	Unit	Source
hf	511.23	kJ/mol	Cheméo Relay (1.0)
hfus	48.05	kJ/mol	Joback Method
hvap	171.29	kJ/mol	Cheméo Relay (1.0)
ie	7.08	eV	NIST Webbook
ie	7.08	eV	NIST Webbook
ie	7.08	eV	NIST Webbook
log10ws	-10.64		Cheméo Relay (1.0)
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
tb	903.63	K	Cheméo Relay (1.0)
tc	1302.90	K	Cheméo Relay (1.0)
tf	627.15	K	Cheméo Relay (1.0)
vc	1.071	m3/kmol	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C190705&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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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