9,10-Anthracenedicarbonitrile

Other names: 9,10-Dicyanoanthracene
9,10-Dicyanoanthracen
Inchi: InChI=1S/C16H8N2/c17-9-15-11-5-1-2-6-12(11)16(10-18)14-8-4-3-7-13(14)15/h1-8H
InchiKey: BIOPPFDHKHWJIA-UHFFFAOYSA-N
Formula: C16H8N2
SMILES: N#Cc1c2ccccc2c(C#N)c2ccccc12
Mol. weight [g/mol]: 228.25
CAS: 1217-45-4

Physical Properties

Property code	Value	Unit	Source
gf	647.02	kJ/mol	Joback Method
hf	540.45	kJ/mol	Joback Method
hfus	27.12	kJ/mol	Joback Method
hvap	79.71	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	3.736		Crippen Method
mcvol	176.380	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	2288.00		NIST Webbook
rinpol	2288.00		NIST Webbook
rinpol	2288.00		NIST Webbook
tb	849.22	K	Joback Method
tc	1112.96	K	Joback Method
tf	529.44	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.63	J/mol×K	849.22	Joback Method
cpg	467.21	J/mol×K	893.18	Joback Method
cpg	476.25	J/mol×K	937.13	Joback Method
cpg	484.90	J/mol×K	981.09	Joback Method

cpg	493.29	J/mol×K	1025.05	Joback Method
cpg	501.58	J/mol×K	1069.00	Joback Method
cpg	509.90	J/mol×K	1112.96	Joback Method

Sources

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=C1217454&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume