

Anthracene, 9,10-diformamido-

Inchi:	InChI=1S/C16H12N2O2/c19-9-17-15-11-5-1-2-6-12(11)16(18-10-20)14-8-4-3-7-13(14)15
InchiKey:	PYSPQAXLYSCIOC-UHFFFAOYSA-N
Formula:	C16H12N2O2
SMILES:	O=CNC1c2ccccc2c(NC=O)c2ccccc12
Mol. weight [g/mol]:	264.28
CAS:	10303-96-5

Physical Properties

Property code	Value	Unit	Source
gf	360.40	kJ/mol	Joback Method
hf	146.47	kJ/mol	Joback Method
hfus	38.88	kJ/mol	Joback Method
hvap	85.06	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.130		Crippen Method
mcvol	196.720	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
tb	842.72	K	Joback Method
tc	1082.81	K	Joback Method
tf	588.78	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.36	J/molxK	842.72	Joback Method
cpg	563.06	J/molxK	882.73	Joback Method
cpg	573.08	J/molxK	922.75	Joback Method
cpg	582.53	J/molxK	962.76	Joback Method
cpg	591.52	J/molxK	1002.78	Joback Method
cpg	600.19	J/molxK	1042.79	Joback Method
cpg	608.64	J/molxK	1082.81	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=C10303965&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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