

aceanthrylene

Inchi:	InChI=1S/C16H10/c1-2-7-14-12(4-1)10-13-6-3-5-11-8-9-15(14)16(11)13/h1-10H
InchiKey:	JDPAVWAQGBGGHD-UHFFFAOYSA-N
Formula:	C16H10
SMILES:	C1=Cc2c3ccccc3cc3cccc1c23
Mol. weight [g/mol]:	202.25
CAS:	202-03-9

Physical Properties

Property code	Value	Unit	Source
gf	491.18	kJ/mol	Joback Method
hf	367.77	kJ/mol	Joback Method
hfus	24.49	kJ/mol	Joback Method
hvap	59.09	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.477		Crippen Method
mcvol	158.460	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinpol	344.20		NIST Webbook
rinpol	341.50		NIST Webbook
tb	651.36	K	Joback Method
tc	907.48	K	Joback Method
tf	425.92	K	Joback Method
vc	0.620	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.64	J/molxK	651.36	Joback Method
cpg	400.96	J/molxK	694.05	Joback Method
cpg	413.12	J/molxK	736.73	Joback Method
cpg	424.36	J/molxK	779.42	Joback Method
cpg	434.86	J/molxK	822.10	Joback Method
cpg	444.86	J/molxK	864.79	Joback Method
cpg	454.56	J/molxK	907.48	Joback Method

dvisc	0.0020100	Paxs	425.92	Joback Method
dvisc	0.0018191	Paxs	463.49	Joback Method
dvisc	0.0016712	Paxs	501.07	Joback Method
dvisc	0.0015536	Paxs	538.64	Joback Method
dvisc	0.0014580	Paxs	576.21	Joback Method
dvisc	0.0013791	Paxs	613.79	Joback Method
dvisc	0.0013128	Paxs	651.36	Joback Method

Sources

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=C202039&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mvol:	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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