

Cyclohept[fg]acenaphthylene

Other names:	Aceplaidylene
Inchi:	InChI=1S/C16H10/c1-2-4-12-6-8-14-10-9-13-7-5-11(3-1)15(12)16(13)14/h1-10H
InchiKey:	NIALEBRUYGMNAY-UHFFFAOYSA-N
Formula:	C16H10
SMILES:	<chem>c1ccc2ccc3ccc4ccc(c1)c2c43</chem>
Mol. weight [g/mol]:	202.25
CAS:	194-32-1

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
ie	7.13 ± 0.04	eV	NIST Webbook
log10ws	-6.30		Crippen Method
logp	4.584		Crippen Method
mcvol	158.460	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
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/mol×K	651.36	Joback Method
cpg	400.96	J/mol×K	694.05	Joback Method
cpg	413.12	J/mol×K	736.73	Joback Method
cpg	424.36	J/mol×K	779.42	Joback Method
cpg	434.86	J/mol×K	822.10	Joback Method
cpg	444.86	J/mol×K	864.79	Joback Method
cpg	454.56	J/mol×K	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=C194321&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
ie:	Ionization energy
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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