

Dibenzo[fg,mn]phenanthro[2,1,10,9,8,7-vwxyza,b]

Inchi:	InChI=1S/C42H20/c1-2-9-24-23(8-1)25-12-5-13-27-31-15-14-22-20-34-28-11-4-7-21-6-3
InchiKey:	KSYHAESVGPXYEH-UHFFFAOYSA-N
Formula:	C42H20
SMILES:	c1ccc2c(c1)c1cccc3c4ccc5cc6c7cccc8cccc(c9ccc%10c%11ccc2c(c13)c%11c4c5c%10c
Mol. weight [g/mol]:	524.61
CAS:	34814-80-7

Physical Properties

Property code	Value	Unit	Source
gf	1468.98	kJ/mol	Joback Method
hf	1131.55	kJ/mol	Joback Method
hfus	73.81	kJ/mol	Joback Method
hvap	133.48	kJ/mol	Joback Method
log10ws	-18.98		Crippen Method
logp	12.123		Crippen Method
mcvol	382.020	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
tb	1414.82	K	Joback Method
tc	1732.17	K	Joback Method
tf	1099.54	K	Joback Method
vc	1.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1608.26	J/molxK	1414.82	Joback Method
cpg	1711.48	J/molxK	1467.71	Joback Method
cpg	1828.85	J/molxK	1520.60	Joback Method
cpg	1961.57	J/molxK	1573.49	Joback Method
cpg	2110.88	J/molxK	1626.39	Joback Method
cpg	2278.00	J/molxK	1679.28	Joback Method
cpg	2464.16	J/molxK	1732.17	Joback Method
dvisc	1.4148251	Paxs	1099.54	Joback Method
dvisc	1.4632370	Paxs	1152.09	Joback Method

dvisc	1.5088701	Paxs	1204.63	Joback Method
dvisc	1.5519371	Paxs	1257.18	Joback Method
dvisc	1.5926328	Paxs	1309.73	Joback Method
dvisc	1.6311352	Paxs	1362.27	Joback Method
dvisc	1.6676068	Paxs	1414.82	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=C34814807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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