

Naph[2,1,8,7:4,10,5]anthra[1,9,8-abcd]coronene

Other names:	Naphth[2',1',8',7':4,10,5]anthra[1,9,8-abcd]coronene
Inchi:	InChI=1S/C38H16/c1-5-19-9-13-23-25-15-11-21-7-3-18-4-8-22-12-16-26-24-14-10-20-6-2
InchiKey:	BEWSIRCXMVBNRU-UHFFFAOYSA-N
Formula:	C38H16
SMILES:	c1cc2ccc3c4ccc5ccc6ccc7ccc8c9ccc%10ccc1c1c2c3c(c9c%101)c1c4c5c6c7c81
Mol. weight [g/mol]:	472.53
CAS:	41163-25-1

Physical Properties

Property code	Value	Unit	Source
gf	1423.78	kJ/mol	Joback Method
hf	1123.19	kJ/mol	Joback Method
hfus	69.40	kJ/mol	Joback Method
hvap	123.30	kJ/mol	Joback Method
ie	6.90	eV	NIST Webbook
ie	6.81 ± 0.02	eV	NIST Webbook
log10ws	-17.81		Crippen Method
logp	10.999		Crippen Method
mcvol	334.260	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
tb	1307.90	K	Joback Method
tc	1603.88	K	Joback Method
tf	1067.02	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1299.53	J/molxK	1307.90	Joback Method
cpg	1378.54	J/molxK	1357.23	Joback Method
cpg	1468.91	J/molxK	1406.56	Joback Method
cpg	1571.69	J/molxK	1455.89	Joback Method
cpg	1687.91	J/molxK	1505.22	Joback Method
cpg	1818.61	J/molxK	1554.55	Joback Method

cpg	1964.83	J/mol×K	1603.88	Joback Method
dvisc	7.8038373	Paxs	1067.02	Joback Method
dvisc	8.3101217	Paxs	1107.17	Joback Method
dvisc	8.8104088	Paxs	1147.31	Joback Method
dvisc	9.3039638	Paxs	1187.46	Joback Method
dvisc	9.7902023	Paxs	1227.61	Joback Method
dvisc	10.2686681	Paxs	1267.75	Joback Method
dvisc	10.7390136	Paxs	1307.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C41163251&Units=SI

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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