Benzo[ghi]naphth[2',1',8',7':5,6,7]aceanthrylene[1

Inchi: InChI=1S/C38H16/c1-2-17-4-5-18-10-11-22-16-26-23-14-12-20-8-6-19-7-9-21-13-15-25-
InchiKey: AFECLTNBDNMWBV-UHFFFAOYSA-N
Formula: C38H16
SMILES: c1cc2ccc3ccc4cc5c6c7c8c-5ccc5ccc9ccc%10ccc(c%11c(c1)c2c3c4c6%11)c7c%10c9c5
Mol. weight [g/mol]: 472.53
CAS: 76748-63-5

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	6.69	eV	NIST Webbook
log10ws	-18.03		Crippen Method
logp	10.950		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/mol×K	1307.90	Joback Method
cpg	1818.61	J/mol×K	1554.55	Joback Method
cpg	1687.91	J/mol×K	1505.22	Joback Method
cpg	1571.69	J/mol×K	1455.89	Joback Method
cpg	1468.91	J/mol×K	1406.56	Joback Method
cpg	1378.54	J/mol×K	1357.23	Joback Method
cpg	1964.83	J/mol×K	1603.88	Joback Method
dvisc	10.7390136	Pa×s	1307.90	Joback Method

dvisc	10.2686681	Pa×s	1267.75	Joback Method
dvisc	9.7902023	Pa×s	1227.61	Joback Method
dvisc	9.3039638	Pa×s	1187.46	Joback Method
dvisc	8.8104088	Pa×s	1147.31	Joback Method
dvisc	8.3101217	Pa×s	1107.17	Joback Method
dvisc	7.8038373	Pa×s	1067.02	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=C76748635&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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