Benzo[a]naphthacene

Inchi: InChI=1S/C22H14/c1-2-7-17-12-20-14-22-18(13-19(20)11-16(17)6-1)10-9-15-5-3-4-8-21(
InchiKey: JTRPLRMCBJSBJV-UHFFFAOYSA-N
Formula: C22H14
SMILES: c1ccc2cc3cc4c(ccc5ccccc54)cc3cc2c1
Mol. weight [g/mol]: 278.35
CAS: 226-88-0

Physical Properties

Property code	Value	Unit	Source
gf	644.48	kJ/mol	Joback Method
hf	468.99	kJ/mol	Joback Method
hfus	33.69	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
ie	7.06 ± 0.04	eV	NIST Webbook
ie	6.74	eV	NIST Webbook
ie	7.03	eV	NIST Webbook
ie	6.97 ± 0.02	eV	NIST Webbook
ie	7.00	eV	NIST Webbook
log10ws	-8.69		Crippen Method
logp	6.299		Crippen Method
mcvol	219.240	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	480.10		NIST Webbook
rinpol	477.70		NIST Webbook
rinpol	500.00		NIST Webbook
tb	820.30	K	Joback Method
tc	1089.89	K	Joback Method
tf	537.00 ± 4.00	K	NIST Webbook
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.64	J/mol×K	820.30	Joback Method

cpg	677.10	J/mol×K	1044.96	Joback Method
cpg	663.56	J/mol×K	1000.03	Joback Method
cpg	650.13	J/mol×K	955.09	Joback Method
cpg	636.52	J/mol×K	910.16	Joback Method
cpg	622.45	J/mol×K	865.23	Joback Method
cpg	691.04	J/mol×K	1089.89	Joback Method
dvisc	0.0011148	Pa×s	820.30	Joback Method
dvisc	0.0012090	Pa×s	772.33	Joback Method
dvisc	0.0013254	Pa×s	724.36	Joback Method
dvisc	0.0014719	Pa×s	676.39	Joback Method
dvisc	0.0016611	Pa×s	628.42	Joback Method
dvisc	0.0019125	Pa×s	580.45	Joback Method
dvisc	0.0022584	Pa×s	532.48	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=C226880&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume