DIBENZ[A,E]ACEANTHRYLENE

Other names: Dibenzo(a,e)fluoranthene
2,3,5,6-Dibenzofluoranthene
Inchi: InChI=1S/C24H14/c1-3-9-17-15(7-1)13-22-19-11-5-6-12-20(19)23-18-10-4-2-8-16(18)14-
InchiKey: JHOWUOKQHJHGMU-UHFFFAOYSA-N
Formula: C24H14
SMILES: c1ccc2c(c1)-c1cc3ccccc3c3cc4ccccc4c-2c13
Mol. weight [g/mol]: 302.38

Physical Properties

Property code	Value	Unit	Source
hf	440.72	kJ/mol	Cheméo Relay (1.0)
hfus	38.47	kJ/mol	Joback Method
hvap	139.79	kJ/mol	Cheméo Relay (1.0)
ie	7.10	eV	Cheméo Relay (1.0)
log10ws	-9.36		Cheméo Relay (1.0)
logp	6.794		Crippen Method
mcvol	232.260	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	535.27		NIST Webbook
rinpol	540.77		NIST Webbook
tb	813.96	K	Cheméo Relay (1.0)
tc	1156.39	K	Cheméo Relay (1.0)
tf	503.07	K	Cheméo Relay (1.0)
vc	0.916	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.36	J/mol×K	1106.54	Joback Method
cpg	757.84	J/mol×K	1151.38	Joback Method
cpg	676.44	J/mol×K	927.16	Joback Method
cpg	691.24	J/mol×K	972.01	Joback Method
cpg	706.42	J/mol×K	1016.85	Joback Method
cpg	722.35	J/mol×K	1061.69	Joback Method

cpg	661.66	J/mol×K	882.32	Joback Method
dvisc	0.0046630	Pa×s	698.45	Joback Method
dvisc	0.0049439	Pa×s	652.49	Joback Method
dvisc	0.0052883	Pa×s	606.52	Joback Method
dvisc	0.0044300	Pa×s	744.42	Joback Method
dvisc	0.0042338	Pa×s	790.39	Joback Method
dvisc	0.0040664	Pa×s	836.35	Joback Method
dvisc	0.0039222	Pa×s	882.32	Joback Method
hfust	24.00	kJ/mol	505.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5385751&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
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