1-BENZYLPYRENE

Inchi:	InChI=1S/C23H16/c1-2-5-16(6-3-1)15-20-12-11-19-10-9-17-7-4-8-18-13-14-21(20)23(19
InchiKey:	KBUVRXNOTZNAPI-UHFFFAOYSA-N
Formula:	C23H16
SMILES:	c1ccc(Cc2ccc3ccc4cccc5ccc2c3c45)cc1
Mol. weight [g/mol]:	292.38

Physical Properties

Property code	Value	Unit	Source
af	0.6517		Cheméo Relay (1.0)
hf	372.27	kJ/mol	Cheméo Relay (1.0)
hfus	36.28	kJ/mol	Joback Method
hvap	125.08	kJ/mol	Cheméo Relay (1.0)
ie	7.51	eV	Cheméo Relay (1.0)
log10ws	-7.79		Cheméo Relay (1.0)
logp	6.175		Crippen Method
mcvol	233.330	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
tb	776.06	K	Cheméo Relay (1.0)
tc	1084.06	K	Cheméo Relay (1.0)
tf	362.15 ± 2.00	K	NIST Webbook
vc	0.899	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.95	J/mol×K	843.18	Joback Method
cpg	750.15	J/mol×K	1106.73	Joback Method
cpg	735.47	J/mol×K	1062.81	Joback Method
cpg	721.21	J/mol×K	1018.88	Joback Method
cpg	707.10	J/mol×K	974.96	Joback Method
cpg	692.87	J/mol×K	931.03	Joback Method
cpg	678.24	J/mol×K	887.11	Joback Method
dvisc	0.0013959	Pa×s	693.47	Joback Method
dvisc	0.0010357	Pa×s	843.18	Joback Method

dvisc	0.0011298	Pa×s	793.28	Joback Method
dvisc	0.0012469	Pa×s	743.37	Joback Method
dvisc	0.0022173	Pa×s	543.75	Joback Method
dvisc	0.0015902	Pa×s	643.56	Joback Method
dvisc	0.0018517	Pa×s	593.65	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42211347&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

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

Latest version available from:
https://www.chemeo.com/cid/18-843-6/1-BENZYLPYRENE.pdf
Generated by Cheméo on 2026-07-21 16:16:54.233900456 +0000 UTC m=+161710.075785846.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.