

9,10-Dibenzylanthracene

Other names:	9,10-Dibenzylanthracene
Inchi:	InChI=1S/C28H22/c1-3-11-21(12-4-1)19-27-23-15-7-9-17-25(23)28(20-22-13-5-2-6-14-2)
InchiKey:	FMVRRCDBALUUBI-UHFFFAOYSA-N
Formula:	C28H22
SMILES:	c1ccc(Cc2c3ccccc3c(Cc3ccccc3)c3ccccc23)cc1
Mol. weight [g/mol]:	358.48

Physical Properties

Property code	Value	Unit	Source
af	0.6932		Cheméo Relay (1.0)
gf	706.52	kJ/mol	Joback Method
hf	426.80	kJ/mol	Cheméo Relay (1.0)
hfus	43.27	kJ/mol	Joback Method
hvap	148.66	kJ/mol	Cheméo Relay (1.0)
ie	7.62	eV	Cheméo Relay (1.0)
log10ws	-9.00		Cheméo Relay (1.0)
logp	7.175		Crippen Method
mcvol	295.180	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
tb	799.51	K	Cheméo Relay (1.0)
tc	1118.10	K	Cheméo Relay (1.0)
tf	451.20	K	Cheméo Relay (1.0)
vc	1.090	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.49	J/mol×K	972.98	Joback Method
cpg	924.11	J/mol×K	1017.81	Joback Method
cpg	940.00	J/mol×K	1062.64	Joback Method
cpg	955.43	J/mol×K	1107.47	Joback Method
cpg	970.65	J/mol×K	1152.30	Joback Method
cpg	985.93	J/mol×K	1197.12	Joback Method
cpg	1001.53	J/mol×K	1241.95	Joback Method

dvisc	0.0007877	Pa×s	587.54	Joback Method
dvisc	0.0005357	Pa×s	651.78	Joback Method
dvisc	0.0003904	Pa×s	716.02	Joback Method
dvisc	0.0002997	Pa×s	780.26	Joback Method
dvisc	0.0002396	Pa×s	844.50	Joback Method
dvisc	0.0001976	Pa×s	908.74	Joback Method
dvisc	0.0001673	Pa×s	972.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3613421&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
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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