

Anthracene, 9-dodecyl-

Other names:	9-Dodecylanthracene 9-n-Dodecylanthracene
Inchi:	InChI=1S/C26H34/c1-2-3-4-5-6-7-8-9-10-11-20-26-24-18-14-12-16-22(24)21-23-17-13-1
InchiKey:	JORZBSFPMKMFMU-UHFFFAOYSA-N
Formula:	C26H34
SMILES:	CCCCCCCCCCCCc1c2ccccc2cc2ccccc12
Mol. weight [g/mol]:	346.55
CAS:	2883-70-7

Physical Properties

Property code	Value	Unit	Source
gf	474.49	kJ/mol	Joback Method
hf	15.76	kJ/mol	Joback Method
hfus	50.40	kJ/mol	Joback Method
hvap	80.35	kJ/mol	Joback Method
log10ws	-10.07		Crippen Method
logp	8.456		Crippen Method
mvol	314.520	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
tb	868.88	K	Joback Method
tc	1081.32	K	Joback Method
tf	322.45 ± 0.50	K	NIST Webbook
vc	1.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.04	J/mol×K	1081.32	Joback Method
cpg	1074.90	J/mol×K	1045.91	Joback Method
cpg	1059.27	J/mol×K	1010.51	Joback Method
cpg	1043.04	J/mol×K	975.10	Joback Method
cpg	1026.10	J/mol×K	939.69	Joback Method
cpg	1008.32	J/mol×K	904.29	Joback Method
cpg	989.60	J/mol×K	868.88	Joback Method

dvisc	0.0010828	Paxs	499.64	Joback Method
dvisc	0.0001824	Paxs	868.88	Joback Method
dvisc	0.0002191	Paxs	807.34	Joback Method
dvisc	0.0002715	Paxs	745.80	Joback Method
dvisc	0.0003494	Paxs	684.26	Joback Method
dvisc	0.0004729	Paxs	622.72	Joback Method
dvisc	0.0006838	Paxs	561.18	Joback Method
hvapt	99.40	kJ/mol	530.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.16848e+01
Coeff. B	-1.03979e+04
Coeff. C	-8.01450e+01
Temperature range (K), min.	566.09
Temperature range (K), max.	715.19

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2883707&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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