

Dibenzo[de,st]pentacene

Inchi:	InChI=1S/C28H16/c1-2-7-19-15-25-20(14-18(19)6-1)16-26-24-11-4-9-17-8-3-10-21(27(1
InchiKey:	DMDCUCGTRMTDIR-UHFFFAOYSA-N
Formula:	C28H16
SMILES:	<chem>c1ccc2cc3c(cc2c1)cc1c2cccc4cccc(c5cccc3c51)c42</chem>
Mol. weight [g/mol]:	352.43
CAS:	14147-38-7

Physical Properties

Property code	Value	Unit	Source
gf	883.28	kJ/mol	Joback Method
hf	658.89	kJ/mol	Joback Method
hfus	45.46	kJ/mol	Joback Method
hvap	92.71	kJ/mol	Joback Method
ie	6.82	eV	NIST Webbook
log10ws	-11.71		Crippen Method
logp	8.044		Crippen Method
mcvol	269.160	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
tb	997.80	K	Joback Method
tc	1271.87	K	Joback Method
tf	696.82	K	Joback Method
vc	1.058	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.33	J/molxK	997.80	Joback Method
cpg	919.98	J/molxK	1226.19	Joback Method
cpg	894.41	J/molxK	1180.51	Joback Method
cpg	871.30	J/molxK	1134.83	Joback Method
cpg	850.20	J/molxK	1089.16	Joback Method
cpg	830.69	J/molxK	1043.48	Joback Method
cpg	948.44	J/molxK	1271.87	Joback Method
dvisc	0.0066304	Paxs	997.80	Joback Method

dvisc	0.0068476	Paxs	947.64	Joback Method
dvisc	0.0070975	Paxs	897.47	Joback Method
dvisc	0.0073878	Paxs	847.31	Joback Method
dvisc	0.0077289	Paxs	797.15	Joback Method
dvisc	0.0081349	Paxs	746.98	Joback Method
dvisc	0.0086256	Paxs	696.82	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=C14147387&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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