Dibenzo[fg,st]pentacene

Inchi: InChI=1S/C28H16/c1-2-8-18-16-26-24-14-6-12-22-20-10-4-3-9-19(20)21-11-5-13-23(27(2
InchiKey: ADWWQMUSHJWMOS-UHFFFAOYSA-N
Formula: C28H16
SMILES: c1ccc2cc3c(cc2c1)c1cccc2c4ccccc4c4cccc3c4c21
Mol. weight [g/mol]: 352.43
CAS: 192-59-6

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	7.33 ± 0.04	eV	NIST Webbook
ie	7.33	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0066304	Pa×s	997.80	Joback Method
dvisc	0.0068476	Pa×s	947.64	Joback Method
dvisc	0.0070975	Pa×s	897.47	Joback Method
dvisc	0.0073878	Pa×s	847.31	Joback Method
dvisc	0.0077289	Pa×s	797.15	Joback Method
dvisc	0.0081349	Pa×s	746.98	Joback Method
dvisc	0.0086256	Pa×s	696.82	Joback Method

Sources

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=C192596&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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