Corannulene

Inchi: InChI=1S/C20H10/c1-2-12-5-6-14-9-10-15-8-7-13-4-3-11(1)16-17(12)19(14)20(15)18(13)
InchiKey: VXRUJZQPKRBJKH-UHFFFAOYSA-N
Formula: C20H10
SMILES: c1cc2ccc3ccc4ccc5ccc1c1c2c3c4c51
Mol. weight [g/mol]: 250.29
CAS: 5821-51-2

Physical Properties

Property code	Value	Unit	Source
gf	707.38	kJ/mol	Joback Method
hf	458.50 ± 9.20	kJ/mol	NIST Webbook
hfs	342.20 ± 6.00	kJ/mol	NIST Webbook
hfus	34.07	kJ/mol	Joback Method
hsub	116.30 ± 7.00	kJ/mol	NIST Webbook
hsub	119.50 ± 4.40	kJ/mol	NIST Webbook
hsub	116.30 ± 6.00	kJ/mol	NIST Webbook
hvap	115.50 ± 2.50	kJ/mol	NIST Webbook
log10ws	-8.74		Crippen Method
logp	5.766		Crippen Method
mcvol	184.500	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	775.40	K	Joback Method
tc	1033.18	K	Joback Method
tf	574.00	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.73	J/mol×K	990.21	Joback Method
cpg	560.60	J/mol×K	1033.18	Joback Method
cpg	488.52	J/mol×K	775.40	Joback Method
cpg	499.82	J/mol×K	818.36	Joback Method
cpg	510.95	J/mol×K	861.33	Joback Method

cpg	522.25	J/mol×K	904.29	Joback Method
cpg	534.06	J/mol×K	947.25	Joback Method
dvisc	0.0154379	Pa×s	775.40	Joback Method
dvisc	0.0150301	Pa×s	741.83	Joback Method
dvisc	0.0125441	Pa×s	574.00	Joback Method
dvisc	0.0131104	Pa×s	607.57	Joback Method
dvisc	0.0136390	Pa×s	641.13	Joback Method
dvisc	0.0141332	Pa×s	674.70	Joback Method
dvisc	0.0145960	Pa×s	708.27	Joback Method
hfust	17.30	kJ/mol	542.30	NIST Webbook
hsubt	115.80	kJ/mol	407.50	NIST Webbook

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=C5821512&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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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