dodecahedrane

Other names: Dodecahedrane
Pentagonal dodecahedrane
Inchi: InChI=1S/C20H20/c1-2-5-7-3(1)9-10-4(1)8-6(2)12-11(5)17-13(7)15(9)19-16(10)14(8)18(1
InchiKey: OOHPORRAEMMMCX-UHFFFAOYSA-N
Formula: C20H20
SMILES: C12C3C4C5C1C1C6C2C2C3C3C4C4C5C1C1C6C2C3C41
Mol. weight [g/mol]: 260.38

Physical Properties

Property code	Value	Unit	Source
affp	843.80	kJ/mol	NIST Webbook
basg	817.50	kJ/mol	NIST Webbook
hf	952.08	kJ/mol	Cheméo Relay (1.0)
hfus	63.98	kJ/mol	Joback Method
hvap	100.80	kJ/mol	Cheméo Relay (1.0)
ie	8.56	eV	Cheméo Relay (1.0)
logp	2.460		Crippen Method
mcvol	173.200	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.22	J/mol×K	633.60	Joback Method
cpg	774.97	J/mol×K	833.77	Joback Method
cpg	758.48	J/mol×K	800.41	Joback Method
cpg	741.77	J/mol×K	767.05	Joback Method
cpg	724.51	J/mol×K	733.68	Joback Method
cpg	706.38	J/mol×K	700.32	Joback Method
cpg	687.06	J/mol×K	666.96	Joback Method
dvisc	107.0544847	Pa×s	576.85	Joback Method
dvisc	399.6504679	Pa×s	633.60	Joback Method
dvisc	264.6826383	Pa×s	614.68	Joback Method
dvisc	170.7679261	Pa×s	595.77	Joback Method
dvisc	21.5123048	Pa×s	520.10	Joback Method

dvisc	65.0206799	Pa×s	557.93	Joback Method
dvisc	38.1327711	Pa×s	539.02	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4493236&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume