

coronene-d12

Inchi:	InChI=1S/C24H12/c1-2-14-5-6-16-9-11-18-12-10-17-8-7-15-4-3-13(1)19-20(14)22(16)24
InchiKey:	VPUGDVKSAQVFFS-AQZSQYOVSAN
Formula:	C24D12
SMILES:	c1cc2ccc3ccc4ccc5ccc6ccc1c1c2c3c4c5c61
Mol. weight [g/mol]:	312.43

Physical Properties

Property code	Value	Unit	Source
gf	838.08	kJ/mol	Joback Method
hf	650.53	kJ/mol	Joback Method
hfus	41.06	kJ/mol	Joback Method
hvap	82.54	kJ/mol	Joback Method
log10ws	-10.54		Crippen Method
logp	6.919		Crippen Method
mvol	221.400	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	549.71		NIST Webbook
rinpol	549.71		NIST Webbook
tb	890.88	K	Joback Method
tc	1154.51	K	Joback Method
tf	664.30	K	Joback Method
vc	0.893	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.52	J/molxK	890.88	Joback Method
cpg	639.68	J/molxK	934.82	Joback Method
cpg	654.66	J/molxK	978.76	Joback Method
cpg	670.86	J/molxK	1022.70	Joback Method
cpg	688.72	J/molxK	1066.64	Joback Method
cpg	708.65	J/molxK	1110.57	Joback Method
cpg	731.08	J/molxK	1154.51	Joback Method
dvisc	0.0266312	Paxs	664.30	Joback Method

dvisc	0.0275768	Paxs	702.06	Joback Method
dvisc	0.0284544	Paxs	739.83	Joback Method
dvisc	0.0292708	Paxs	777.59	Joback Method
dvisc	0.0300317	Paxs	815.35	Joback Method
dvisc	0.0307426	Paxs	853.12	Joback Method
dvisc	0.0314079	Paxs	890.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R394599&Units=SI
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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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