

Pentacyclo[3.3.3.0^{2,4}.0^{6,8}

Other names: Pentacyclo[3.3.3.0^{2,4}.0^{6,8}
Stereoisomer
Inchi: InChI=1S/C11H14/c1-4-5(1)11-7-2-6(7)10(4)8-3-9(8)11/h4-11H,1-3H2
InchiKey: TZRQBQARGUABOE-UHFFFAOYSA-N
Formula: C11H14
SMILES: C1C2C1C1C3CC3C2C2CC21
Mol. weight [g/mol]: 146.23
CAS: 70469-89-5

Physical Properties

Property code	Value	Unit	Source
gf	370.76	kJ/mol	Joback Method
hf	57.25	kJ/mol	Joback Method
hfus	26.53	kJ/mol	Joback Method
hvap	38.03	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-1.97		Crippen Method
logp	2.154		Crippen Method
mcvol	111.550	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	453.69	K	Joback Method
tc	656.71	K	Joback Method
tf	304.79	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.40	J/molxK	453.69	Joback Method
cpg	377.36	J/molxK	622.87	Joback Method
cpg	362.97	J/molxK	589.04	Joback Method
cpg	347.32	J/molxK	555.20	Joback Method
cpg	330.28	J/molxK	521.36	Joback Method
cpg	311.69	J/molxK	487.53	Joback Method

cpg	390.67	J/molxK	656.71	Joback Method
dvisc	0.0079106	Paxs	453.69	Joback Method
dvisc	0.0055142	Paxs	428.87	Joback Method
dvisc	0.0036770	Paxs	404.06	Joback Method
dvisc	0.0023253	Paxs	379.24	Joback Method
dvisc	0.0013791	Paxs	354.42	Joback Method
dvisc	0.0007560	Paxs	329.61	Joback Method
dvisc	0.0003758	Paxs	304.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70469895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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