Pentacyclo[3.3.3.0^{2,4}.0<sup>6,8</su stereoisomer

Other names: Pentacyclo[3.3.3.0

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	8.60	eV	NIST Webbook
ie	8.80	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/mol×K	453.69	Joback Method
cpg	311.69	J/mol×K	487.53	Joback Method
cpg	330.28	J/mol×K	521.36	Joback Method
cpg	347.32	J/mol×K	555.20	Joback Method
cpg	362.97	J/mol×K	589.04	Joback Method
cpg	377.36	J/mol×K	622.87	Joback Method

cpg	390.67	J/mol×K	656.71	Joback Method
dvisc	0.0003758	Pa×s	304.79	Joback Method
dvisc	0.0007560	Pa×s	329.61	Joback Method
dvisc	0.0013791	Pa×s	354.42	Joback Method
dvisc	0.0023253	Pa×s	379.24	Joback Method
dvisc	0.0036770	Pa×s	404.06	Joback Method
dvisc	0.0055142	Pa×s	428.87	Joback Method
dvisc	0.0079106	Pa×s	453.69	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=C70469895&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

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