Pentacyclo[6.3.1.13,6.02,7.09,11]tridecane

Other names:	Pentacyclo[6.3.1.1
Inchi:	InChI=1S/C13H18/c1-2-7-3-6(1)12-10-5-11(13(7)12)9-4-8(9)10/h6-13H,1-5H2
InchiKey:	KONJIGRBVREIQG-UHFFFAOYSA-N
Formula:	C13H18
SMILES:	C1CC2CC1C1C3CC(C4CC43)C21
Mol. weight [g/mol]:	174.28
CAS:	61140-68-9

Physical Properties

Property code	Value	Unit	Source
chl	-7713.90 ± 3.80	kJ/mol	NIST Webbook
gf	363.40	kJ/mol	Joback Method
hf	3.65	kJ/mol	Joback Method
hfl	25.80 ± 3.80	kJ/mol	NIST Webbook
hfus	27.51	kJ/mol	Joback Method
hvap	42.83	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.934		Crippen Method
mcvol	139.730	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
tb	507.99	K	Joback Method
tc	720.91	K	Joback Method
tf	320.29	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.98	J/mol×K	507.99	Joback Method
cpg	411.84	J/mol×K	543.48	Joback Method
cpg	432.92	J/mol×K	578.96	Joback Method
cpg	452.38	J/mol×K	614.45	Joback Method
cpg	470.39	J/mol×K	649.94	Joback Method
cpg	487.11	J/mol×K	685.43	Joback Method

cpg	502.71	J/mol×K	720.91	Joback Method
dvisc	0.0009709	Pa×s	320.29	Joback Method
dvisc	0.0017962	Pa×s	351.57	Joback Method
dvisc	0.0030052	Pa×s	382.86	Joback Method
dvisc	0.0046518	Pa×s	414.14	Joback Method
dvisc	0.0067721	Pa×s	445.42	Joback Method
dvisc	0.0093846	Pa×s	476.71	Joback Method
dvisc	0.0124927	Pa×s	507.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61140689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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