

Tetrapiro[2.0.0.0.2.1.1.1]undecane

Inchi: InChI=1S/C11H14/c1-2-8(1)5-10(8)7-11(10)6-9(11)3-4-9/h1-7H2
InchiKey: JISOCMQWQHEYKJ-UHFFFAOYSA-N
Formula: C11H14
SMILES: C1CC12CC21CC12CC21CC1
Mol. weight [g/mol]: 146.23
CAS: 129872-30-6

Physical Properties

Property code	Value	Unit	Source
chl	-6818.00 ± 6.60	kJ/mol	NIST Webbook
gf	379.64	kJ/mol	Joback Method
hf	544.00 ± 6.80	kJ/mol	NIST Webbook
hfl	488.60 ± 6.80	kJ/mol	NIST Webbook
hfus	-2.94	kJ/mol	Joback Method
hvap	55.40 ± 0.40	kJ/mol	NIST Webbook
hvap	55.40	kJ/mol	NIST Webbook
log10ws	-2.93		Crippen Method
logp	2.731		Crippen Method
mcvol	111.550	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
tb	473.33	K	Joback Method
tc	716.92	K	Joback Method
tf	417.35	K	Joback Method
vc	0.462	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.93	J/mol×K	473.33	Joback Method
cpg	313.05	J/mol×K	513.93	Joback Method
cpg	328.77	J/mol×K	554.53	Joback Method
cpg	341.88	J/mol×K	595.12	Joback Method
cpg	353.16	J/mol×K	635.72	Joback Method
cpg	363.40	J/mol×K	676.32	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C129872306&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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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