

1-epi-«alpha»-Pinguisene

Inchi:	InChI=1S/C15H24/c1-6-13-8-10-14(4)11(2)7-9-15(14,5)12(13)3/h6,8,11-12H,1,7,9-10H2,
InchiKey:	PFLVCUHFTYXGSL-VIRABCJISA-N
Formula:	C15H24
SMILES:	C=CC1=CCC2(C)C(C)CCC2(C)C1C
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	242.39	kJ/mol	Joback Method
hf	-64.27	kJ/mol	Joback Method
hfus	13.68	kJ/mol	Joback Method
hvap	46.69	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	1370.00		NIST Webbook
tb	560.85	K	Joback Method
tc	782.69	K	Joback Method
tf	334.97	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.68	J/mol×K	560.85	Joback Method
cpg	520.18	J/mol×K	597.82	Joback Method
cpg	541.23	J/mol×K	634.80	Joback Method
cpg	561.06	J/mol×K	671.77	Joback Method
cpg	579.93	J/mol×K	708.74	Joback Method
cpg	598.08	J/mol×K	745.71	Joback Method
cpg	615.75	J/mol×K	782.69	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=R425079&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
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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