

Striatene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24/c1-6-12(2)10-11-15(5)13(3)8-7-9-14(15)4/h6,8,10,14H,1,7,9,11H2,2-5

SDGBQFYFDSSQI-INXSZFJKSA-N

C15H24

C=CC(C)=CCC1(C)C(C)=CCCC1C

204.35

Physical Properties

Property code	Value	Unit	Source
gf	266.51	kJ/mol	Joback Method
hf	-24.54	kJ/mol	Joback Method
hfus	19.66	kJ/mol	Joback Method
hvap	48.28	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.891		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	1461.00		NIST Webbook
tb	562.58	K	Joback Method
tc	773.72	K	Joback Method
tf	278.33	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.69	J/mol×K	562.58	Joback Method
cpg	513.72	J/mol×K	597.77	Joback Method
cpg	533.52	J/mol×K	632.96	Joback Method
cpg	552.22	J/mol×K	668.15	Joback Method
cpg	569.94	J/mol×K	703.34	Joback Method
cpg	586.82	J/mol×K	738.53	Joback Method
cpg	602.99	J/mol×K	773.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R431386&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

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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