

1-Propyl-2-methyl-trans-2-hexyl-cyclopropane

Inchi:	InChI=1S/C13H26/c1-4-6-7-8-10-13(3)11-12(13)9-5-2/h12H,4-11H2,1-3H3/t12-,13-/m1/s
InchiKey:	VORAYVNJSRJQJJ-CHWSQXEVSA-N
Formula:	C13H26
SMILES:	CCCCCCC1(C)CC1CCC
Mol. weight [g/mol]:	182.35

Physical Properties

Property code	Value	Unit	Source
gf	106.13	kJ/mol	Joback Method
hf	-243.95	kJ/mol	Joback Method
hfus	22.33	kJ/mol	Joback Method
hvap	42.98	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.783		Crippen Method
mcvol	183.170	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1198.60		NIST Webbook
rinpol	1198.60		NIST Webbook
tb	499.15	K	Joback Method
tc	676.75	K	Joback Method
tf	273.87	K	Joback Method
vc	0.718	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.67	J/molxK	499.15	Joback Method
cpg	461.68	J/molxK	528.75	Joback Method
cpg	479.69	J/molxK	558.35	Joback Method
cpg	496.79	J/molxK	587.95	Joback Method
cpg	513.05	J/molxK	617.55	Joback Method
cpg	528.56	J/molxK	647.15	Joback Method
cpg	543.39	J/molxK	676.75	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=R137638&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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