1-Hexyl-2-methyl-cis-2-propyl-cyclopropane

Inchi: InChI=1S/C13H26/c1-4-6-7-8-9-12-11-13(12,3)10-5-2/h12H,4-11H2,1-3H3/t12-,13+/m1/s
InchiKey: DTINIVGEKVRRTJ-OLZOCXBDSA-N
Formula: C13H26
SMILES: CCCCCCC1CC1(C)CCC
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	1214.40		NIST Webbook
tb	499.15	K	Joback Method
tc	676.75	K	Joback Method
tf	273.87	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.67	J/mol×K	499.15	Joback Method
cpg	461.68	J/mol×K	528.75	Joback Method
cpg	479.69	J/mol×K	558.35	Joback Method
cpg	496.79	J/mol×K	587.95	Joback Method
cpg	513.05	J/mol×K	617.55	Joback Method
cpg	528.56	J/mol×K	647.15	Joback Method
cpg	543.39	J/mol×K	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=R137158&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
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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