1-ethyl-trans-2-hexyl-cyclopropane

Inchi: InChI=1S/C11H22/c1-3-5-6-7-8-11-9-10(11)4-2/h10-11H,3-9H2,1-2H3/t10-,11-/m1/s1
InchiKey: YPODGGYYHXRDLB-GHMZBOCLSA-N
Formula: C11H22
SMILES: CCCCCCC1CC1CC
Mol. weight [g/mol]: 154.29

Physical Properties

Property code	Value	Unit	Source
gf	94.78	kJ/mol	Joback Method
hf	-217.91	kJ/mol	Joback Method
hfus	23.45	kJ/mol	Joback Method
hvap	39.68	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	4.003		Crippen Method
mcvol	154.990	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1057.90		NIST Webbook
rinpol	1056.60		NIST Webbook
tb	453.15	K	Joback Method
tc	626.88	K	Joback Method
tf	227.43	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.16	J/mol×K	453.15	Joback Method
cpg	363.74	J/mol×K	482.11	Joback Method
cpg	380.53	J/mol×K	511.06	Joback Method
cpg	396.58	J/mol×K	540.02	Joback Method
cpg	411.90	J/mol×K	568.97	Joback Method
cpg	426.54	J/mol×K	597.93	Joback Method
cpg	440.50	J/mol×K	626.88	Joback Method
dvisc	0.0014603	Pa×s	227.43	Joback Method

dvisc	0.0010151	Pa×s	265.05	Joback Method
dvisc	0.0007724	Pa×s	302.67	Joback Method
dvisc	0.0006243	Pa×s	340.29	Joback Method
dvisc	0.0005265	Pa×s	377.91	Joback Method
dvisc	0.0004579	Pa×s	415.53	Joback Method
dvisc	0.0004076	Pa×s	453.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R137123&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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