2-Propyn-1-ol, 1,1-dicyclopropyl-

Inchi: InChI=1S/C9H12O/c1-2-9(10,7-3-4-7)8-5-6-8/h1,7-8,10H,3-6H2
InchiKey: OXBOSLIINGKALV-UHFFFAOYSA-N
Formula: C9H12O
SMILES: C#CC(O)(C1CC1)C1CC1
Mol. weight [g/mol]: 136.19
CAS: 24297-12-9

Physical Properties

Property code	Value	Unit	Source
gf	235.49	kJ/mol	Joback Method
hf	47.43	kJ/mol	Joback Method
hfus	14.98	kJ/mol	Joback Method
hvap	50.70	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.171		Crippen Method
mcvol	113.220	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
tb	497.87	K	Joback Method
tc	705.02	K	Joback Method
tf	337.28	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.42	J/mol×K	497.87	Joback Method
cpg	288.33	J/mol×K	532.39	Joback Method
cpg	301.11	J/mol×K	566.92	Joback Method
cpg	312.86	J/mol×K	601.44	Joback Method
cpg	323.68	J/mol×K	635.97	Joback Method
cpg	333.66	J/mol×K	670.49	Joback Method
cpg	342.89	J/mol×K	705.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24297129&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume