

Cyclobutyl ethynyl methyl carbinol

Inchi:	InChI=1S/C8H12O/c1-3-8(2,9)7-5-4-6-7/h1,7,9H,4-6H2,2H3
InchiKey:	OOQOQWCONGHTDA-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	C#CC(C)(O)C1CCC1
Mol. weight [g/mol]:	124.18
CAS:	515-81-1

Physical Properties

Property code	Value	Unit	Source
gf	154.22	kJ/mol	Joback Method
hf	-10.89	kJ/mol	Joback Method
hfus	12.16	kJ/mol	Joback Method
hvap	48.73	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.171		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	472.52	K	Joback Method
tc	674.33	K	Joback Method
tf	304.55	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.52	J/molxK	472.52	Joback Method
cpg	258.52	J/molxK	506.15	Joback Method
cpg	270.62	J/molxK	539.79	Joback Method
cpg	281.88	J/molxK	573.42	Joback Method
cpg	292.35	J/molxK	607.06	Joback Method
cpg	302.10	J/molxK	640.69	Joback Method
cpg	311.17	J/molxK	674.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C515811&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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