3-Cyclopentyl-1-propyne

Other names: Cyclopentylpropyne
2-propynylcyclopentane
Inchi: InChI=1S/C8H12/c1-2-5-8-6-3-4-7-8/h1,8H,3-7H2
InchiKey: VBTCAHMANZTRMG-UHFFFAOYSA-N
Formula: C8H12
SMILES: C#CCC1CCCC1
Mol. weight [g/mol]: 108.18
CAS: 116279-08-4

Physical Properties

Property code	Value	Unit	Source
gf	276.10	kJ/mol	Joback Method
hf	143.93	kJ/mol	Joback Method
hfus	13.39	kJ/mol	Joback Method
hvap	33.52	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.200		Crippen Method
mcvol	104.120	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
tb	387.84	K	Joback Method
tc	595.39	K	Joback Method
tf	237.79	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.65	J/mol×K	387.84	Joback Method
cpg	202.81	J/mol×K	422.43	Joback Method
cpg	217.12	J/mol×K	457.02	Joback Method
cpg	230.61	J/mol×K	491.62	Joback Method
cpg	243.33	J/mol×K	526.21	Joback Method
cpg	255.30	J/mol×K	560.80	Joback Method
cpg	266.57	J/mol×K	595.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116279084&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

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