1-Cyclopropylpenta-1,3-diyne

Inchi: InChI=1S/C8H8/c1-2-3-4-5-8-6-7-8/h8H,6-7H2,1H3
InchiKey: ZEKLXAZDDKNQBK-UHFFFAOYSA-N
Formula: C8H8
SMILES: CC#CC#CC1CC1
Mol. weight [g/mol]: 104.15
CAS: 116316-76-8

Physical Properties

Property code	Value	Unit	Source
chl	-4724.20 ± 8.00	kJ/mol	NIST Webbook
gf	482.83	kJ/mol	Joback Method
hf	484.70	kJ/mol	NIST Webbook
hfl	432.80 ± 8.00	kJ/mol	NIST Webbook
hfus	20.86	kJ/mol	Joback Method
hvap	51.90 ± 0.10	kJ/mol	NIST Webbook
hvap	51.90	kJ/mol	NIST Webbook
hvap	51.90	kJ/mol	NIST Webbook
log10ws	-2.41		Crippen Method
logp	1.423		Crippen Method
mcvol	95.520	ml/mol	McGowan Method
pc	4238.55	kPa	Joback Method
tb	407.18	K	Joback Method
tc	642.80	K	Joback Method
tf	410.06	K	Joback Method
vc	0.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.33	J/mol×K	407.18	Joback Method
cpg	178.52	J/mol×K	446.45	Joback Method
cpg	189.92	J/mol×K	485.72	Joback Method
cpg	200.57	J/mol×K	524.99	Joback Method
cpg	210.53	J/mol×K	564.26	Joback Method

cpg	219.85	J/mol×K	603.53	Joback Method
cpg	228.58	J/mol×K	642.80	Joback Method

Sources

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=C116316768&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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