CH3-CC-CC-CH2

Inchi: InChI=1S/C6H5/c1-3-5-6-4-2/h1H2,2H3
InchiKey: TZTSOMWOQWNAND-UHFFFAOYSA-N
Formula: C6H5
SMILES: [CH2]C#CC#CC
Mol. weight [g/mol]: 77.10
CAS: 116138-99-9

Physical Properties

Property code	Value	Unit	Source
affp	819.10	kJ/mol	NIST Webbook
basg	786.60	kJ/mol	NIST Webbook
gf	457.62	kJ/mol	Joback Method
hf	433.24	kJ/mol	Joback Method
hfus	19.22	kJ/mol	Joback Method
hvap	33.11	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	0.847		Crippen Method
mcvol	76.050	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
tb	353.98	K	Joback Method
tc	569.21	K	Joback Method
tf	385.95	K	Joback Method
vc	0.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	110.51	J/mol×K	353.98	Joback Method
cpg	117.25	J/mol×K	389.85	Joback Method
cpg	123.52	J/mol×K	425.72	Joback Method
cpg	129.38	J/mol×K	461.59	Joback Method
cpg	134.84	J/mol×K	497.46	Joback Method
cpg	139.96	J/mol×K	533.33	Joback Method
cpg	144.76	J/mol×K	569.21	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=C116138999&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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