HCCCH2CH()CCH

Inchi: InChI=1S/C6H5/c1-3-5-6-4-2/h1-2,5H,6H2
InchiKey: UMFJGJFSNKBCNL-UHFFFAOYSA-N
Formula: C6H5
SMILES: C#C[CH]CC#C
Mol. weight [g/mol]: 77.10
CAS: 116139-00-5

Physical Properties

Property code	Value	Unit	Source
affp	748.90	kJ/mol	NIST Webbook
basg	716.40	kJ/mol	NIST Webbook
gf	495.72	kJ/mol	Joback Method
hf	467.16	kJ/mol	Joback Method
hfus	15.40	kJ/mol	Joback Method
hvap	28.13	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	0.847		Crippen Method
mcvol	76.050	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	315.78	K	Joback Method
tc	505.14	K	Joback Method
tf	252.69	K	Joback Method
vc	0.281	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.31	J/mol×K	315.78	Joback Method
cpg	122.50	J/mol×K	347.34	Joback Method
cpg	129.10	J/mol×K	378.90	Joback Method
cpg	135.17	J/mol×K	410.46	Joback Method
cpg	140.73	J/mol×K	442.02	Joback Method
cpg	145.83	J/mol×K	473.58	Joback Method
cpg	150.50	J/mol×K	505.14	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116139005&Units=SI

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

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