1,3-Pentadiyne

Inchi: InChI=1S/C5H4/c1-3-5-4-2/h1H,2H3
InchiKey: VNMDYSSJFJFEQI-UHFFFAOYSA-N
Formula: C5H4
SMILES: C#CC#CC
Mol. weight [g/mol]: 64.09
CAS: 4911-55-1

Physical Properties

Property code	Value	Unit	Source
gf	417.09	kJ/mol	Joback Method
hf	417.67	kJ/mol	Joback Method
hfus	14.80	kJ/mol	Joback Method
hvap	28.73	kJ/mol	Joback Method
ie	9.51	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.50 ± 0.02	eV	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.51	eV	NIST Webbook
log10ws	-1.50		Crippen Method
logp	0.643		Crippen Method
mcvol	64.110	ml/mol	McGowan Method
pc	5175.72	kPa	Joback Method
tb	328.00 ± 4.00	K	NIST Webbook
tb	328.70	K	NIST Webbook
tc	516.81	K	Joback Method
tf	299.18	K	Joback Method
vc	0.239	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	89.77	J/mol×K	312.92	Joback Method
cpg	94.86	J/mol×K	346.90	Joback Method
cpg	99.71	J/mol×K	380.88	Joback Method

cpg	104.32	J/mol×K	414.87	Joback Method
cpg	108.72	J/mol×K	448.85	Joback Method
cpg	112.91	J/mol×K	482.83	Joback Method
cpg	116.90	J/mol×K	516.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4911551&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
ie:	Ionization energy
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