(E)-2-Pentenenitrile

Other names: 2-Pentenenitrile, (E)-
(E)-pent-2-enenitrile
Inchi: InChI=1S/C5H7N/c1-2-3-4-5-6/h3-4H,2H2,1H3/b4-3+
InchiKey: ISBHMJZRKAFTGE-ONEGZZNKSA-N
Formula: C5H7N
SMILES: CCC=CC#N
Mol. weight [g/mol]: 81.12
CAS: 26294-98-4

Physical Properties

Property code	Value	Unit	Source
chl	-3042.90 ± 1.00	kJ/mol	NIST Webbook
gf	204.62	kJ/mol	Joback Method
hf	119.70 ± 1.00	kJ/mol	NIST Webbook
hfl	74.90 ± 1.00	kJ/mol	NIST Webbook
hfus	10.41	kJ/mol	Joback Method
hvap	44.90 ± 0.20	kJ/mol	NIST Webbook
hvap	44.90	kJ/mol	NIST Webbook
hvap	44.80	kJ/mol	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.476		Crippen Method
mcvol	78.390	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	420.04	K	Joback Method
tc	620.58	K	Joback Method
tf	206.02	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.82	J/mol×K	420.04	Joback Method
cpg	144.23	J/mol×K	453.46	Joback Method
cpg	151.25	J/mol×K	486.89	Joback Method

cpg	157.88	J/mol×K	520.31	Joback Method
cpg	164.16	J/mol×K	553.73	Joback Method
cpg	170.09	J/mol×K	587.15	Joback Method
cpg	175.70	J/mol×K	620.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26294984&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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