but-2(E)-enenitrile

Other names: (E)-2-Butenenitrile
Inchi: InChI=1S/C4H5N/c1-2-3-4-5/h2-3H,1H3/b3-2+
InchiKey: NKKMVIVFRUYPLQ-NSCUHMNNSA-N
Formula: C4H5N
SMILES: CC=CC#N
Mol. weight [g/mol]: 67.09
CAS: 627-26-9

Physical Properties

Property code	Value	Unit	Source
chl	-2389.30 ± 0.88	kJ/mol	NIST Webbook
chl	-2393.00	kJ/mol	NIST Webbook
gf	196.20	kJ/mol	Joback Method
hf	140.70 ± 0.92	kJ/mol	NIST Webbook
hfl	100.70 ± 0.92	kJ/mol	NIST Webbook
hfus	7.82	kJ/mol	Joback Method
hvap	40.00	kJ/mol	NIST Webbook
hvap	40.00	kJ/mol	NIST Webbook
hvap	40.00	kJ/mol	NIST Webbook
ie	10.23 ± 0.05	eV	NIST Webbook
log10ws	-1.22		Crippen Method
logp	1.086		Crippen Method
mcvol	64.300	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
rinpol	637.00		NIST Webbook
rinpol	637.00		NIST Webbook
ripol	1157.00		NIST Webbook
ripol	1157.00		NIST Webbook
tb	397.16	K	Joback Method
tc	599.62	K	Joback Method
tf	194.75	K	Joback Method
vc	0.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.11	J/mol×K	532.13	Joback Method
cpg	128.76	J/mol×K	565.87	Joback Method
cpg	102.51	J/mol×K	397.16	Joback Method
cpg	108.39	J/mol×K	430.90	Joback Method
cpg	113.94	J/mol×K	464.65	Joback Method
cpg	119.18	J/mol×K	498.39	Joback Method
cpg	133.16	J/mol×K	599.62	Joback Method
hvapt	39.70	kJ/mol	356.00	NIST Webbook
hvapt	40.50	kJ/mol	324.50	NIST Webbook

Sources

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=C627269&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure

rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume