Butanenitrile, 2-methylene-

Other names:	Butyronitrile, 2-methylene-
	«alpha»-Ethylacrylonitrile
	2-Ethylacrylonitrile
	2-Methylenebutyronitrile
	2-Propenenitrile, 2-ethyl-
Inchi:	InChI=1S/C5H7N/c1-3-5(2)4-6/h2-3H2,1H3
InchiKey:	TVONJMOVBKMLOM-UHFFFAOYSA-N
Formula:	C5H7N
SMILES:	C=C(C#N)CC
Mol. weight [g/mol]:	81.12
CAS:	1647-11-6

Physical Properties

Property code	Value	Unit	Source
gf	203.69	kJ/mol	Joback Method
hf	133.99	kJ/mol	Joback Method
hfus	7.62	kJ/mol	Joback Method
hvap	36.61	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.476		Crippen Method
mcvol	78.390	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
tb	412.44	K	Joback Method
tc	611.25	K	Joback Method
tf	195.38	K	Joback Method
vc	0.324	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.97	J/mol×K	578.11	Joback Method
cpg	138.02	J/mol×K	412.44	Joback Method
cpg	145.29	J/mol×K	445.57	Joback Method
cpg	152.21	J/mol×K	478.71	Joback Method

cpg	158.78	J/mol×K	511.84	Joback Method
cpg	165.03	J/mol×K	544.98	Joback Method
cpg	176.61	J/mol×K	611.25	Joback Method
hvapt	37.10	kJ/mol	315.50	NIST Webbook

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=C1647116&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
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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