

CIS-CROTONITRILE

Other names:	(E)-2-BUTENENITRILE
Inchi:	InChI=1S/C4H9N/c1-2-3-4-5/h2-3H,4-5H2,1H3
InchiKey:	QFUSOYKIDBRREL-NSCUHMNNSA-N
Formula:	C4H9N
SMILES:	CC=CCN
Mol. weight [g/mol]:	67.09
CAS:	1190-76-7

Physical Properties

Property code	Value	Unit	Source
gf	129.47	kJ/mol	Joback Method
hf	25.12	kJ/mol	Joback Method
hfus	11.51	kJ/mol	Joback Method
hvap	35.10	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.521		Crippen Method
mcvol	72.900	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	380.62	K	KDB
tc	559.28	K	Joback Method
tf	213.02	K	Joback Method
vc	0.269	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.09	J/mol×K	367.61	Joback Method
cpg	132.44	J/mol×K	399.56	Joback Method
cpg	140.37	J/mol×K	431.50	Joback Method
cpg	147.89	J/mol×K	463.45	Joback Method
cpg	155.02	J/mol×K	495.39	Joback Method
cpg	161.79	J/mol×K	527.34	Joback Method
cpg	168.21	J/mol×K	559.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1403

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
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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