

2-Butenoic acid, 2-cyano-3-methyl-, ethyl ester

Other names:	Crotonic acid, 2-cyano-3-methyl-, ethyl ester Ethyl isopropylidene(cyano)acetate Ethyl 2-cyano-3-methylcrotonate
Inchi:	InChI=1S/C8H11NO2/c1-4-11-8(10)7(5-9)6(2)3/h4H2,1-3H3
InchiKey:	PZMDAADKKAXROL-UHFFFAOYSA-N
Formula:	C8H11NO2
SMILES:	CCOC(=O)C(C#N)=C(C)C
Mol. weight [g/mol]:	153.18
CAS:	759-58-0

Physical Properties

Property code	Value	Unit	Source
gf	-21.14	kJ/mol	Joback Method
hf	-190.73	kJ/mol	Joback Method
hfus	18.35	kJ/mol	Joback Method
hvap	53.15	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.409		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
tb	564.73	K	Joback Method
tc	772.90	K	Joback Method
tf	284.07	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.68	J/molxK	564.73	Joback Method
cpg	300.03	J/molxK	599.42	Joback Method
cpg	309.85	J/molxK	634.12	Joback Method
cpg	319.15	J/molxK	668.81	Joback Method
cpg	327.95	J/molxK	703.51	Joback Method
cpg	336.26	J/molxK	738.20	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	371.70	K	0.10	NIST Webbook
tbrp	394.50 ± 1.50	K	2.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C759580&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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