2-Butene, 2-amino-3-cyano-

Inchi: InChI=1S/C5H8N2/c1-4(3-6)5(2)7/h7H2,1-2H3/b5-4-
InchiKey: KSBIPDJRJJHHFE-PLNGDYQASA-N
Formula: C5H8N2
SMILES: CC(N)=C(C)C#N
Mol. weight [g/mol]: 96.13
CAS: 19483-78-4

Physical Properties

Property code	Value	Unit	Source
gf	253.97	kJ/mol	Joback Method
hf	149.78	kJ/mol	Joback Method
hfus	12.99	kJ/mol	Joback Method
hvap	47.96	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	0.763		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
tb	492.33	K	Joback Method
tc	714.19	K	Joback Method
tf	261.36	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.96	J/mol×K	492.33	Joback Method
cpg	188.10	J/mol×K	529.31	Joback Method
cpg	195.74	J/mol×K	566.28	Joback Method
cpg	202.91	J/mol×K	603.26	Joback Method
cpg	209.64	J/mol×K	640.23	Joback Method
cpg	215.96	J/mol×K	677.21	Joback Method
cpg	221.91	J/mol×K	714.19	Joback Method

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=C19483784&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
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