(BUTYLAMINO)ACETONITRILE

Other names: N-n-Butylaminoacetonitrile
(n-Butylamino)acetonitrile
Acetonitrile, (butylamino)-
Inchi: InChI=1S/C6H12N2/c1-2-3-5-8-6-4-7/h8H,2-3,5-6H2,1H3
InchiKey: SPMMZKAWNAKPJM-UHFFFAOYSA-N
Formula: C6H12N2
SMILES: CCCCNCC#N
Mol. weight [g/mol]: 112.18

Physical Properties

Property code	Value	Unit	Source
af	0.5064		Cheméo Relay (1.0)
hf	46.51	kJ/mol	Cheméo Relay (1.0)
hfus	17.90	kJ/mol	Joback Method
hvap	53.06	kJ/mol	Cheméo Relay (1.0)
ie	9.12	eV	Cheméo Relay (1.0)
log10ws	-0.51		Cheméo Relay (1.0)
logp	0.900		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	469.10	K	Cheméo Relay (1.0)
tc	638.15	K	Cheméo Relay (1.0)
tf	218.11	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.14	J/mol×K	488.93	Joback Method
cpg	240.07	J/mol×K	520.87	Joback Method
cpg	249.55	J/mol×K	552.81	Joback Method
cpg	258.59	J/mol×K	584.76	Joback Method
cpg	267.21	J/mol×K	616.70	Joback Method
cpg	275.42	J/mol×K	648.64	Joback Method
cpg	283.23	J/mol×K	680.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.20	K	1.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3010046&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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