Acetonitrile, bromo-

Other names: Bromoacetonitrile
Bromomethyl cyanide
Cyanomethyl bromide
Inchi: InChI=1S/C2H2BrN/c3-1-2-4/h1H2
InchiKey: REXUYBKPWIPONM-UHFFFAOYSA-N
Formula: C2H2BrN
SMILES: N#CCBr
Mol. weight [g/mol]: 119.95
CAS: 590-17-0

Physical Properties

Property code	Value	Unit	Source
gf	113.46	kJ/mol	Joback Method
hf	106.60	kJ/mol	Joback Method
hfus	7.73	kJ/mol	Joback Method
hvap	36.96	kJ/mol	Joback Method
ie	11.28	eV	NIST Webbook
log10ws	-0.96		Crippen Method
logp	0.905		Crippen Method
mcvol	57.920	ml/mol	McGowan Method
pc	5359.18	kPa	Joback Method
rinpol	725.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	725.00		NIST Webbook
tb	413.40	K	Joback Method
tc	629.95	K	Joback Method
tf	237.09	K	Joback Method
vc	0.235	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	76.64	J/mol×K	413.40	Joback Method
cpg	79.57	J/mol×K	449.49	Joback Method

cpg	82.31	J/mol×K	485.58	Joback Method
cpg	84.88	J/mol×K	521.67	Joback Method
cpg	87.29	J/mol×K	557.76	Joback Method
cpg	89.55	J/mol×K	593.86	Joback Method
cpg	91.67	J/mol×K	629.95	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	334.20	K	3.20	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C590170&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume