«beta»-Butylaminoisobutyronitrile

Inchi: InChI=1S/C8H16N2/c1-3-4-5-10-7-8(2)6-9/h8,10H,3-5,7H2,1-2H3
InchiKey: YEOFLJMHUKTFBH-UHFFFAOYSA-N
Formula: C8H16N2
SMILES: CCCCNCC(C)C#N
Mol. weight [g/mol]: 140.23
CAS: 63145-02-8

Physical Properties

Property code	Value	Unit	Source
chl	-5356.30 ± 3.40	kJ/mol	NIST Webbook
gf	236.61	kJ/mol	Joback Method
hf	4.62	kJ/mol	Joback Method
hfl	-78.50 ± 3.40	kJ/mol	NIST Webbook
hfus	19.56	kJ/mol	Joback Method
hvap	49.93	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.536		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
tb	534.25	K	Joback Method
tc	725.29	K	Joback Method
tf	282.57	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.85	J/mol×K	534.25	Joback Method
cpg	329.10	J/mol×K	566.09	Joback Method
cpg	340.78	J/mol×K	597.93	Joback Method
cpg	351.90	J/mol×K	629.77	Joback Method
cpg	362.48	J/mol×K	661.61	Joback Method
cpg	372.54	J/mol×K	693.45	Joback Method
cpg	382.09	J/mol×K	725.29	Joback Method

Sources

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=C63145028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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