3,4-Epoxybutyl cyanide

Inchi: InChI=1S/C5H7NO/c6-3-1-2-5-4-7-5/h5H,1-2,4H2
InchiKey: DRZQOARGLZRJBN-UHFFFAOYSA-N
Formula: C5H7NO
SMILES: N#CCCC1CO1
Mol. weight [g/mol]: 97.12

Physical Properties

Property code	Value	Unit	Source
gf	99.03	kJ/mol	Joback Method
hf	-40.85	kJ/mol	Joback Method
hfus	16.33	kJ/mol	Joback Method
hvap	41.62	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	0.689		Crippen Method
mcvol	77.700	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
ripol	1863.00		NIST Webbook
ripol	1863.00		NIST Webbook
tb	449.57	K	Joback Method
tc	656.34	K	Joback Method
tf	255.61	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.31	J/mol×K	449.57	Joback Method
cpg	170.02	J/mol×K	484.03	Joback Method
cpg	178.19	J/mol×K	518.49	Joback Method
cpg	185.84	J/mol×K	552.96	Joback Method
cpg	193.00	J/mol×K	587.42	Joback Method
cpg	199.72	J/mol×K	621.88	Joback Method
cpg	206.01	J/mol×K	656.34	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=R586862&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume