«alpha»-Chloroisovaleronitrile

Inchi: InChI=1S/C5H8ClN/c1-4(2)5(6)3-7/h4-5H,1-2H3
InchiKey: GMPPCOCINGLLFH-UHFFFAOYSA-N
Formula: C5H8ClN
SMILES: CC(C)C(Cl)C#N
Mol. weight [g/mol]: 117.58
CAS: 70477-21-3

Physical Properties

Property code	Value	Unit	Source
gf	107.59	kJ/mol	Joback Method
hf	-7.95	kJ/mol	Joback Method
hfus	7.36	kJ/mol	Joback Method
hvap	40.81	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.773		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	452.43	K	Joback Method
tc	659.33	K	Joback Method
tf	211.02	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.11	J/mol×K	452.43	Joback Method
cpg	183.26	J/mol×K	486.91	Joback Method
cpg	190.99	J/mol×K	521.40	Joback Method
cpg	198.34	J/mol×K	555.88	Joback Method
cpg	205.30	J/mol×K	590.36	Joback Method
cpg	211.89	J/mol×K	624.85	Joback Method
cpg	218.12	J/mol×K	659.33	Joback Method

Sources

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=C70477213&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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