isobutyl cyanoacetate

Inchi: InChI=1S/C7H11NO2/c1-6(2)5-10-7(9)3-4-8/h6H,3,5H2,1-2H3
InchiKey: HRGQEKKNLHJZGZ-UHFFFAOYSA-N
Formula: C7H11NO2
SMILES: CC(C)COC(=O)CC#N
Mol. weight [g/mol]: 141.17
CAS: 13361-31-4

Physical Properties

Property code	Value	Unit	Source
gf	-95.12	kJ/mol	Joback Method
hf	-273.01	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	50.42	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	1.099		Crippen Method
mcvol	118.310	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
tb	537.49	K	Joback Method
tc	736.93	K	Joback Method
tf	290.80	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.90	J/mol×K	537.49	Joback Method
cpg	275.82	J/mol×K	570.73	Joback Method
cpg	285.31	J/mol×K	603.97	Joback Method
cpg	294.37	J/mol×K	637.21	Joback Method
cpg	302.99	J/mol×K	670.45	Joback Method
cpg	311.17	J/mol×K	703.69	Joback Method
cpg	318.92	J/mol×K	736.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13361314&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
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