Methyl(n-cyanomethyl-n-methyl)-beta-aminopropi

Inchi: InChI=1S/C7H12N2O2/c1-9(6-4-8)5-3-7(10)11-2/h3,5-6H2,1-2H3
InchiKey: OISXPVIXWOLSPB-UHFFFAOYSA-N
Formula: C7H12N2O2
SMILES: COC(=O)CCN(C)CC#N
Mol. weight [g/mol]: 156.18
CAS: 59039-83-7

Physical Properties

Property code	Value	Unit	Source
gf	18.10	kJ/mol	Joback Method
hf	-200.20	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-0.05		Crippen Method
logp	0.005		Crippen Method
mcvol	128.290	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
tb	550.37	K	Joback Method
tc	743.28	K	Joback Method
tf	338.27	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.91	J/mol×K	550.37	Joback Method
cpg	309.34	J/mol×K	582.52	Joback Method
cpg	319.27	J/mol×K	614.67	Joback Method
cpg	328.71	J/mol×K	646.82	Joback Method
cpg	337.67	J/mol×K	678.97	Joback Method
cpg	346.15	J/mol×K	711.13	Joback Method
cpg	354.18	J/mol×K	743.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59039837&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

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