Methyl 1,2,3,6-tetrahydropyridine-3-carboxylate

Inchi: InChI=1S/C7H11NO2/c1-10-7(9)6-3-2-4-8-5-6/h2-3,6,8H,4-5H2,1H3
InchiKey: UQTWITUUILHZFF-UHFFFAOYSA-N
Formula: C7H11NO2
SMILES: COC(=O)C1C=CCNC1
Mol. weight [g/mol]: 141.17
CAS: 121743-23-5

Physical Properties

Property code	Value	Unit	Source
gf	-83.74	kJ/mol	Joback Method
hf	-282.70	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	47.81	kJ/mol	Joback Method
log10ws	-0.31		Crippen Method
logp	-0.065		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
rinpol	1164.20		NIST Webbook
rinpol	1164.20		NIST Webbook
tb	503.11	K	Joback Method
tc	726.09	K	Joback Method
tf	353.98	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.74	J/mol×K	503.11	Joback Method
cpg	258.73	J/mol×K	540.27	Joback Method
cpg	272.01	J/mol×K	577.44	Joback Method
cpg	284.60	J/mol×K	614.60	Joback Method
cpg	296.48	J/mol×K	651.76	Joback Method
cpg	307.65	J/mol×K	688.93	Joback Method
cpg	318.12	J/mol×K	726.09	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=C121743235&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume