Guvacoline

Inchi: InChI=1S/C7H11NO2/c1-10-7(9)6-3-2-4-8-5-6/h3,8H,2,4-5H2,1H3
InchiKey: DYPLDWLIOGXSSE-UHFFFAOYSA-N
Formula: C7H11NO2
SMILES: COC(=O)C1=CCCNC1
Mol. weight [g/mol]: 141.17
CAS: 495-19-2

Physical Properties

Property code	Value	Unit	Source
gf	-85.66	kJ/mol	Joback Method
hf	-273.83	kJ/mol	Joback Method
hfus	17.86	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.079		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	1250.30		NIST Webbook
rinpol	1250.30		NIST Webbook
tb	512.76	K	Joback Method
tc	737.11	K	Joback Method
tf	370.74	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.38	J/mol×K	512.76	Joback Method
cpg	256.60	J/mol×K	550.15	Joback Method
cpg	269.16	J/mol×K	587.54	Joback Method
cpg	281.06	J/mol×K	624.94	Joback Method
cpg	292.30	J/mol×K	662.33	Joback Method
cpg	302.86	J/mol×K	699.72	Joback Method
cpg	312.76	J/mol×K	737.11	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C495192&Units=SI

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