Guvacine ethyl ester

Inchi: InChI=1S/C8H13NO2/c1-2-11-8(10)7-4-3-5-9-6-7/h4,9H,2-3,5-6H2,1H3
InchiKey: DBJSKLKTQJMDTJ-UHFFFAOYSA-N
Formula: C8H13NO2
SMILES: CCOC(=O)C1=CCCNC1
Mol. weight [g/mol]: 155.19
CAS: 18513-76-3

Physical Properties

Property code	Value	Unit	Source
gf	-77.24	kJ/mol	Joback Method
hf	-294.47	kJ/mol	Joback Method
hfus	20.45	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.469		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	1324.50		NIST Webbook
rinpol	1324.50		NIST Webbook
tb	535.64	K	Joback Method
tc	756.09	K	Joback Method
tf	382.01	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.75	J/mol×K	535.64	Joback Method
cpg	302.03	J/mol×K	572.38	Joback Method
cpg	315.57	J/mol×K	609.12	Joback Method
cpg	328.39	J/mol×K	645.87	Joback Method
cpg	340.49	J/mol×K	682.61	Joback Method
cpg	351.85	J/mol×K	719.35	Joback Method
cpg	362.50	J/mol×K	756.09	Joback Method

Sources

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=C18513763&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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