4-Methoxycarbonylmethyl-4,5-dihydro-1H-pyrazol acid methyl ester

Inchi: InChI=1S/C8H12N2O4/c1-13-6(11)3-5-4-9-10-7(5)8(12)14-2/h5,9H,3-4H2,1-2H3

InchiKey: DZJMFGBPMRRUGK-UHFFFAOYSA-N

Formula: C8H12N2O4

SMILES: COC(=O)CC1CNN=C1C(=O)OC

Mol. weight [g/mol]: 200.19

Physical Properties

Property code	Value	Unit	Source
gf	-189.99	kJ/mol	Joback Method
hf	-482.48	kJ/mol	Joback Method
hfus	31.55	kJ/mol	Joback Method
hvap	65.89	kJ/mol	Joback Method
log10ws	0.11		Crippen Method
logp	-0.702		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
rinpol	1598.00		NIST Webbook
tb	656.69	K	Joback Method
tc	881.36	K	Joback Method
tf	524.99	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.27	J/mol×K	656.69	Joback Method
cpg	405.09	J/mol×K	694.13	Joback Method
cpg	418.03	J/mol×K	731.58	Joback Method
cpg	430.06	J/mol×K	769.02	Joback Method
cpg	441.15	J/mol×K	806.47	Joback Method
cpg	451.25	J/mol×K	843.91	Joback Method
cpg	460.32	J/mol×K	881.36	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=R249424&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