4-(2-Methoxycarbonyl-ethyl)-4,5-dihydro-1H-pyraz
acid methyl ester

Inchi: InChI=1S/C9H14N2O4/c1-14-7(12)4-3-6-5-10-11-8(6)9(13)15-2/h6,10H,3-5H2,1-2H3
InchiKey: XKZJHNIBPKFLQK-UHFFFAOYSA-N
Formula: C9H14N2O4
SMILES: COC(=O)CCC1CNN=C1C(=O)OC
Mol. weight [g/mol]: 214.22

Physical Properties

Property code	Value	Unit	Source
gf	-181.57	kJ/mol	Joback Method
hf	-503.12	kJ/mol	Joback Method
hfus	34.14	kJ/mol	Joback Method
hvap	68.12	kJ/mol	Joback Method
log10ws	-0.31		Crippen Method
logp	-0.312		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
rinpol	1720.00		NIST Webbook
tb	679.57	K	Joback Method
tc	900.27	K	Joback Method
tf	536.26	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.08	J/mol×K	679.57	Joback Method
cpg	456.48	J/mol×K	716.35	Joback Method
cpg	469.93	J/mol×K	753.14	Joback Method
cpg	482.42	J/mol×K	789.92	Joback Method
cpg	493.90	J/mol×K	826.70	Joback Method
cpg	504.34	J/mol×K	863.48	Joback Method
cpg	513.72	J/mol×K	900.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249380&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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