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

Inchi: InChI=1S/C11H18N2O4/c1-16-9(14)6-4-3-5-8-7-12-13-10(8)11(15)17-2/h8,12H,3-7H2,1-
InchiKey: UQSAMDBHMYOZNC-UHFFFAOYSA-N
Formula: C11H18N2O4
SMILES: COC(=O)CCCCC1CNN=C1C(=O)OC
Mol. weight [g/mol]: 242.27

Physical Properties

Property code	Value	Unit	Source
gf	-164.73	kJ/mol	Joback Method
hf	-544.40	kJ/mol	Joback Method
hfus	39.32	kJ/mol	Joback Method
hvap	72.57	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	0.468		Crippen Method
mcvol	185.530	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
tb	725.33	K	Joback Method
tc	939.25	K	Joback Method
tf	558.80	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.69	J/mol×K	725.33	Joback Method
cpg	562.93	J/mol×K	760.98	Joback Method
cpg	577.12	J/mol×K	796.64	Joback Method
cpg	590.23	J/mol×K	832.29	Joback Method
cpg	602.23	J/mol×K	867.94	Joback Method
cpg	613.10	J/mol×K	903.60	Joback Method
cpg	622.83	J/mol×K	939.25	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=R249404&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