4-(3-Methoxycarbonyl-propyl)-4,5-dihydro-1H-pyra
acid methyl ester

Inchi: InChI=1S/C10H16N2O4/c1-15-8(13)5-3-4-7-6-11-12-9(7)10(14)16-2/h7,11H,3-6H2,1-2H3

InchiKey: KJPWAOVLRCILTP-UHFFFAOYSA-N

Formula: C10H16N2O4

SMILES: COC(=O)CCCC1CNN=C1C(=O)OC

Mol. weight [g/mol]: 228.25

Physical Properties

Property code	Value	Unit	Source
gf	-173.15	kJ/mol	Joback Method
hf	-523.76	kJ/mol	Joback Method
hfus	36.73	kJ/mol	Joback Method
hvap	70.34	kJ/mol	Joback Method
log10ws	-0.73		Crippen Method
logp	0.078		Crippen Method
mcvol	171.440	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
tb	702.45	K	Joback Method
tc	919.55	K	Joback Method
tf	547.53	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.25	J/mol×K	702.45	Joback Method
cpg	509.12	J/mol×K	738.63	Joback Method
cpg	522.99	J/mol×K	774.82	Joback Method
cpg	535.83	J/mol×K	811.00	Joback Method
cpg	547.61	J/mol×K	847.18	Joback Method
cpg	558.31	J/mol×K	883.37	Joback Method
cpg	567.89	J/mol×K	919.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249395&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

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