4,5-Dihydro-1H-pyrazole-3,4-dicarboxylic acid dimethyl ester

Inchi: InChI=1S/C7H10N2O4/c1-12-6(10)4-3-8-9-5(4)7(11)13-2/h4,8H,3H2,1-2H3
InchiKey: HDHXZOHSNQOFNR-UHFFFAOYSA-N
Formula: C7H10N2O4
SMILES: COC(=O)C1=NNCC1C(=O)OC
Mol. weight [g/mol]: 186.17

Physical Properties

Property code	Value	Unit	Source
gf	-198.41	kJ/mol	Joback Method
hf	-461.84	kJ/mol	Joback Method
hfus	28.96	kJ/mol	Joback Method
hvap	63.67	kJ/mol	Joback Method
log10ws	0.53		Crippen Method
logp	-1.092		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
tb	633.81	K	Joback Method
tc	862.79	K	Joback Method
tf	513.72	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.94	J/mol×K	633.81	Joback Method
cpg	355.04	J/mol×K	671.97	Joback Method
cpg	367.34	J/mol×K	710.14	Joback Method
cpg	378.81	J/mol×K	748.30	Joback Method
cpg	389.40	J/mol×K	786.46	Joback Method
cpg	399.06	J/mol×K	824.62	Joback Method
cpg	407.75	J/mol×K	862.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249419&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