Cyclopentanecarboxamide, 2,3-dihydroxy-4-(hydroxymethyl)-2,3-diacetate

Inchi: InChI=1S/C11H17NO6/c1-5(14)17-9-7(4-13)3-8(11(12)16)10(9)18-6(2)15/h7-10,13H,3-4

InchiKey: NNHXSJPQECUWBQ-UHFFFAOYSA-N

Formula: C11H17NO6

SMILES: CC(=O)OC1C(CO)CC(C(N)=O)C1OC(C)=O

Mol. weight [g/mol]: 259.26

CAS: 13190-79-9

Physical Properties

Property code	Value	Unit	Source
gf	-611.97	kJ/mol	Joback Method
hf	-991.53	kJ/mol	Joback Method
hfus	37.85	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-0.26		Crippen Method
logp	-1.036		Crippen Method
mcvol	187.290	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	823.51	K	Joback Method
tc	1029.71	K	Joback Method
tf	550.24	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.62	J/mol×K	823.51	Joback Method
cpg	611.35	J/mol×K	857.88	Joback Method
cpg	622.06	J/mol×K	892.24	Joback Method
cpg	631.72	J/mol×K	926.61	Joback Method
cpg	640.32	J/mol×K	960.98	Joback Method
cpg	647.86	J/mol×K	995.34	Joback Method
cpg	654.33	J/mol×K	1029.71	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=C13190799&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume