exo-Bicyclo[2.2.1]hept-5-en-2-carboxylic acid, 2-methyl, methyl ester

Inchi: InChI=1S/C10H14O2/c1-10(9(11)12-2)6-7-3-4-8(10)5-7/h3-4,7-8H,5-6H2,1-2H3/t7-,8+,10

InchiKey: AEBDJCUTXUYLDC-QXFUBDJGSA-N

Formula: C10H14O2

SMILES: COC(=O)C1(C)CC2C=CC1C2

Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	-74.44	kJ/mol	Joback Method
hf	-302.41	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	45.84	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.762		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1480.00		NIST Webbook
tb	516.97	K	Joback Method
tc	733.38	K	Joback Method
tf	327.40	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.49	J/mol×K	516.97	Joback Method
cpg	339.57	J/mol×K	553.04	Joback Method
cpg	354.50	J/mol×K	589.11	Joback Method
cpg	368.43	J/mol×K	625.17	Joback Method
cpg	381.47	J/mol×K	661.24	Joback Method
cpg	393.78	J/mol×K	697.31	Joback Method

cpg	405.49	J/mol×K	733.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R13197&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume