exo-Bicyclo[2.2.1]hept-5-en-2-carboxylic acid, 7,7-cyclopropano-2-methyl, methyl ester

Inchi: InChI=1S/C12H16O2/c1-11(10(13)14-2)7-8-3-4-9(11)12(8)5-6-12/h3-4,8-9H,5-7H2,1-2H3

InchiKey: UPOPHKONFXCKPW-WCABBAIRSA-N

Formula: C12H16O2

SMILES: COC(=O)C1(C)CC2C=CC1C21CC1

Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	9.76	kJ/mol	Joback Method
hf	-249.49	kJ/mol	Joback Method
hfus	13.72	kJ/mol	Joback Method
hvap	48.88	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.152		Crippen Method
mcvol	150.500	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
rinpol	1254.00		NIST Webbook
rinpol	1254.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1614.00		NIST Webbook
tb	565.44	K	Joback Method
tc	791.70	K	Joback Method
tf	395.30	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.36	J/mol×K	565.44	Joback Method
cpg	419.21	J/mol×K	603.15	Joback Method
cpg	434.74	J/mol×K	640.86	Joback Method
cpg	449.27	J/mol×K	678.57	Joback Method
cpg	463.09	J/mol×K	716.28	Joback Method
cpg	476.51	J/mol×K	753.99	Joback Method

cpg	489.83	J/mol×K	791.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R13204&Units=SI

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