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

Inchi: InChI=1S/C11H14O2/c1-13-10(12)8-6-7-2-3-9(8)11(7)4-5-11/h2-3,7-9H,4-6H2,1H3/t7-,8-

InchiKey: MYPALZWZXZILKP-HLTSFMKQSA-N

Formula: C11H14O2

SMILES: COC(=O)C1CC2C=CC1C21CC1

Mol. weight [g/mol]: 178.23

Physical Properties

Property code	Value	Unit	Source
gf	6.83	kJ/mol	Joback Method
hf	-244.09	kJ/mol	Joback Method
hfus	17.43	kJ/mol	Joback Method
hvap	47.81	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.762		Crippen Method
mcvol	136.410	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	1230.00		NIST Webbook
ripol	1643.00		NIST Webbook
tb	542.32	K	Joback Method
tc	763.54	K	Joback Method
tf	360.13	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.54	J/mol×K	542.32	Joback Method
cpg	372.18	J/mol×K	579.19	Joback Method
cpg	387.52	J/mol×K	616.06	Joback Method
cpg	401.74	J/mol×K	652.93	Joback Method
cpg	415.04	J/mol×K	689.80	Joback Method
cpg	427.61	J/mol×K	726.67	Joback Method
cpg	439.62	J/mol×K	763.54	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=R13218&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
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