endo-Bicyclo[2.2.1]heptan-2-carboxylic acid, 7,7-cyclopropano, methyl ester

Inchi: InChI=1S/C11H16O2/c1-13-10(12)8-6-7-2-3-9(8)11(7)4-5-11/h7-9H,2-6H2,1H3/t7-,8+,9+

InchiKey: BOBIGPLBAPRCGC-VGMNWLOBSA-N

Formula: C11H16O2

SMILES: COC(=O)C1CC2CCC1C21CC1

Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	-23.13	kJ/mol	Joback Method
hf	-301.87	kJ/mol	Joback Method
hfus	16.21	kJ/mol	Joback Method
hvap	47.52	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.986		Crippen Method
mcvol	140.710	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	1268.00		NIST Webbook
rinpol	1268.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1643.00		NIST Webbook
tb	543.16	K	Joback Method
tc	762.22	K	Joback Method
tf	359.37	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.14	J/mol×K	543.16	Joback Method
cpg	391.98	J/mol×K	579.67	Joback Method
cpg	408.48	J/mol×K	616.18	Joback Method
cpg	423.84	J/mol×K	652.69	Joback Method
cpg	438.23	J/mol×K	689.20	Joback Method
cpg	451.84	J/mol×K	725.71	Joback Method

cpg	464.85	J/mol×K	762.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R13165&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

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