Bicyclo[2.2.2]octan-1-carboxylic acid, methyl ester

Inchi: InChI=1S/C10H16O2/c1-12-9(11)10-5-2-8(3-6-10)4-7-10/h8H,2-7H2,1H3
InchiKey: ZZQHNCFQLQSTAS-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: COC(=O)C12CCC(CC1)CC2
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-108.79	kJ/mol	Joback Method
hf	-346.01	kJ/mol	Joback Method
hfus	10.21	kJ/mol	Joback Method
hvap	46.03	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.130		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	1247.00		NIST Webbook
rinpol	1247.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1631.00		NIST Webbook
tb	526.75	K	Joback Method
tc	749.18	K	Joback Method
tf	327.36	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.63	J/mol×K	526.75	Joback Method
cpg	358.44	J/mol×K	563.82	Joback Method
cpg	374.99	J/mol×K	600.89	Joback Method
cpg	390.43	J/mol×K	637.96	Joback Method
cpg	404.90	J/mol×K	675.04	Joback Method
cpg	418.56	J/mol×K	712.11	Joback Method

cpg	431.55	J/mol×K	749.18	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=R13062&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