exo-Bicyclo[2.2.1]heptan-2-carboxylic acid, 2-methyl, methyl ester

Inchi: InChI=1S/C10H16O2/c1-10(9(11)12-2)6-7-3-4-8(10)5-7/h7-8H,3-6H2,1-2H3/t7-,8+,10+/m

InchiKey: AINYFZUYWPYGJW-WEDXCCLWSA-N

Formula: C10H16O2

SMILES: COC(=O)C1(C)CC2CCC1C2

Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-104.40	kJ/mol	Joback Method
hf	-360.19	kJ/mol	Joback Method
hfus	13.39	kJ/mol	Joback Method
hvap	45.55	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.986		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
rinpol	1156.00		NIST Webbook
ripol	1488.00		NIST Webbook
tb	517.81	K	Joback Method
tc	732.08	K	Joback Method
tf	326.64	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.10	J/mol×K	517.81	Joback Method
cpg	358.39	J/mol×K	553.52	Joback Method
cpg	374.50	J/mol×K	589.23	Joback Method
cpg	389.56	J/mol×K	624.95	Joback Method
cpg	403.72	J/mol×K	660.66	Joback Method
cpg	417.10	J/mol×K	696.37	Joback Method
cpg	429.83	J/mol×K	732.08	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=R13240&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