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

Inchi: InChI=1S/C12H18O2/c1-11(10(13)14-2)7-8-3-4-9(11)12(8)5-6-12/h8-9H,3-7H2,1-2H3/t8-

InchiKey: BYBXYWJLTXNRDH-WCABBAIRSA-N

Formula: C12H18O2

SMILES: COC(=O)C1(C)CC2CCC1C21CC1

Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	-20.20	kJ/mol	Joback Method
hf	-307.27	kJ/mol	Joback Method
hfus	12.50	kJ/mol	Joback Method
hvap	48.59	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.376		Crippen Method
mcvol	154.800	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1291.00		NIST Webbook
ripol	1623.00		NIST Webbook
tb	566.28	K	Joback Method
tc	790.33	K	Joback Method
tf	394.54	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.85	J/mol×K	566.28	Joback Method
cpg	439.88	J/mol×K	603.62	Joback Method
cpg	456.57	J/mol×K	640.96	Joback Method
cpg	472.22	J/mol×K	678.31	Joback Method
cpg	487.11	J/mol×K	715.65	Joback Method
cpg	501.54	J/mol×K	752.99	Joback Method
cpg	515.81	J/mol×K	790.33	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=R13254&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

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