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

Inchi: InChI=1S/C11H18O2/c1-11(2)7-4-5-9(11)8(6-7)10(12)13-3/h7-9H,4-6H2,1-3H3/t7-,8-,9+/

InchiKey: YOEDQIUFJQMKBL-HLTSFMKQSA-N

Formula: C11H18O2

SMILES: COC(=O)C1CC2CCC1C2(C)C

Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	-103.69	kJ/mol	Joback Method
hf	-401.17	kJ/mol	Joback Method
hfus	17.05	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.232		Crippen Method
mcvol	151.570	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1268.00		NIST Webbook
rinpol	1268.00		NIST Webbook
ripol	1635.00		NIST Webbook
tb	536.02	K	Joback Method
tc	746.72	K	Joback Method
tf	333.67	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.61	J/mol×K	536.02	Joback Method
cpg	407.93	J/mol×K	571.14	Joback Method
cpg	425.11	J/mol×K	606.25	Joback Method
cpg	441.27	J/mol×K	641.37	Joback Method
cpg	456.53	J/mol×K	676.49	Joback Method
cpg	471.02	J/mol×K	711.60	Joback Method
cpg	484.85	J/mol×K	746.72	Joback Method

Sources

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=R13272&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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