(6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl)methyl ethyl carbonate

InchI: InChI=1S/C13H20O3/c1-4-15-12(14)16-8-9-5-6-10-7-11(9)13(10,2)3/h5,10-11H,4,6-8H2,
InchiKey: FXUQWEPTCASLSK-UHFFFAOYSA-N
Formula: C13H20O3
SMILES: CCOC(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 224.30

Physical Properties

Property code	Value	Unit	Source
gf	-163.81	kJ/mol	Joback Method
hf	-508.02	kJ/mol	Joback Method
hfus	23.18	kJ/mol	Joback Method
hvap	55.59	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	3.152		Crippen Method
mcvol	181.320	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1499.00		NIST Webbook
tb	613.01	K	Joback Method
tc	818.04	K	Joback Method
tf	395.96	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.85	J/mol×K	613.01	Joback Method
cpg	512.89	J/mol×K	647.18	Joback Method
cpg	529.06	J/mol×K	681.35	Joback Method
cpg	544.45	J/mol×K	715.53	Joback Method
cpg	559.19	J/mol×K	749.70	Joback Method
cpg	573.36	J/mol×K	783.87	Joback Method
cpg	587.09	J/mol×K	818.04	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=U373804&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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