Ethyl (1R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl carbonate

Inchi: InChI=1S/C13H22O3/c1-5-15-11(14)16-10-8-9-6-7-13(10,4)12(9,2)3/h9-10H,5-8H2,1-4H
InchiKey: LIQVUHGCRXJZDF-UHFFFAOYSA-N
Formula: C13H22O3
SMILES: CCOC(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	-197.34	kJ/mol	Joback Method
hf	-559.43	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	53.18	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.374		Crippen Method
mcvol	185.620	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1461.00		NIST Webbook
rinpol	1461.00		NIST Webbook
tb	604.44	K	Joback Method
tc	814.19	K	Joback Method
tf	402.34	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.21	J/mol×K	604.44	Joback Method
cpg	534.76	J/mol×K	639.40	Joback Method
cpg	552.36	J/mol×K	674.36	Joback Method
cpg	569.22	J/mol×K	709.31	Joback Method
cpg	585.51	J/mol×K	744.27	Joback Method
cpg	601.42	J/mol×K	779.23	Joback Method
cpg	617.15	J/mol×K	814.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373772&Units=SI
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

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