4-(2,7,7-Trimethylbicyclo[3.2.0]hept-2-en-1-yl)but-

Other names: 4-(2',7',7'-Trimethyl-bicyclo[3.2.0]hept-2'-en-1'-yl)but-3-en-2-one
Inchi: InChI=1S/C14H20O/c1-10-5-6-12-9-13(3,4)14(10,12)8-7-11(2)15/h5,7-8,12H,6,9H2,1-4H
InchiKey: ZXVDYQWETIMVLL-FPLPWBNLSA-N
Formula: C14H20O
SMILES: CC(=O)C=CC12C(C)=CCC1CC2(C)C
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
gf	129.34	kJ/mol	Joback Method
hf	-131.76	kJ/mol	Joback Method
hfus	17.29	kJ/mol	Joback Method
hvap	51.80	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.514		Crippen Method
mcvol	179.370	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1472.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1472.00		NIST Webbook
tb	595.45	K	Joback Method
tc	818.73	K	Joback Method
tf	381.59	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.23	J/mol×K	595.45	Joback Method
cpg	487.97	J/mol×K	632.66	Joback Method
cpg	504.61	J/mol×K	669.88	Joback Method
cpg	520.43	J/mol×K	707.09	Joback Method
cpg	535.69	J/mol×K	744.30	Joback Method
cpg	550.69	J/mol×K	781.52	Joback Method

cpg	565.70	J/mol×K	818.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U195437&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