(1S,4R,5R)-1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octa acetate

Inchi: InChI=1S/C12H20O3/c1-8(13)14-10-7-12(4)6-5-9(10)11(2,3)15-12/h9-10H,5-7H2,1-4H3
InchiKey: LUYHJKNQBUWCNY-UHFFFAOYSA-N
Formula: C12H20O3
SMILES: CC(=O)OC1CC2(C)CCC1C(C)(C)O2
Mol. weight [g/mol]: 212.29
CAS: 81781-24-0

Physical Properties

Property code	Value	Unit	Source
gf	-198.98	kJ/mol	Joback Method
hf	-544.73	kJ/mol	Joback Method
hfus	19.22	kJ/mol	Joback Method
hvap	53.22	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.286		Crippen Method
mcvol	171.530	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
rinpol	1343.40		NIST Webbook
rinpol	1343.40		NIST Webbook
tb	590.36	K	Joback Method
tc	811.40	K	Joback Method
tf	391.89	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.00	J/mol×K	590.36	Joback Method
cpg	490.68	J/mol×K	627.20	Joback Method
cpg	508.27	J/mol×K	664.04	Joback Method
cpg	525.00	J/mol×K	700.88	Joback Method
cpg	541.09	J/mol×K	737.72	Joback Method
cpg	556.75	J/mol×K	774.56	Joback Method
cpg	572.21	J/mol×K	811.40	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=C81781240&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