

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

Inchi: InChI=1S/C10H18O2/c1-9(2)7-4-5-10(3,12-9)6-8(7)11/h7-8,11H,4-6H2,1-3H3
InchiKey: WHIKIYRWRMRQNK-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC12CCC(C(O)C1)C(C)(C)O2
Mol. weight [g/mol]: 170.25
CAS: 81801-58-3

Physical Properties

Property code	Value	Unit	Source
gf	-118.72	kJ/mol	Joback Method
hf	-410.88	kJ/mol	Joback Method
hfus	15.34	kJ/mol	Joback Method
hvap	56.29	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.715		Crippen Method
mcvol	141.780	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1259.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1240.70		NIST Webbook
rinpol	1240.70		NIST Webbook
ripol	2160.00		NIST Webbook
ripol	2160.00		NIST Webbook
tb	560.49	K	Joback Method
tc	767.10	K	Joback Method
tf	358.01	K	Joback Method
vc	0.527	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.49	J/mol×K	560.49	Joback Method
cpg	402.41	J/mol×K	594.92	Joback Method
cpg	417.30	J/mol×K	629.36	Joback Method

cpg	431.35	J/mol×K	663.79	Joback Method
cpg	444.77	J/mol×K	698.23	Joback Method
cpg	457.73	J/mol×K	732.66	Joback Method
cpg	470.44	J/mol×K	767.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C81801583&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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