1,5,5-Trimethyl-9-oxa-bicyclo[4.3.0]non-2-ene

Inchi: InChI=1S/C11H18O/c1-10(2)6-4-7-11(3)9(10)5-8-12-11/h4,7,9H,5-6,8H2,1-3H3
InchiKey: ZVMRRDREWREYBC-UHFFFAOYSA-N
Formula: C11H18O
SMILES: CC1(C)CC=CC2(C)OCCC12
Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	52.09	kJ/mol	Joback Method
hf	-207.33	kJ/mol	Joback Method
hfus	11.89	kJ/mol	Joback Method
hvap	42.61	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.768		Crippen Method
mcvol	145.700	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1168.50		NIST Webbook
rinpol	1168.50		NIST Webbook
tb	499.29	K	Joback Method
tc	729.16	K	Joback Method
tf	309.94	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.03	J/mol×K	499.29	Joback Method
cpg	372.39	J/mol×K	537.60	Joback Method
cpg	391.04	J/mol×K	575.91	Joback Method
cpg	408.25	J/mol×K	614.23	Joback Method
cpg	424.29	J/mol×K	652.54	Joback Method
cpg	439.42	J/mol×K	690.85	Joback Method
cpg	453.92	J/mol×K	729.16	Joback Method

Sources

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=R416258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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