(1R,4R,5S)-1-Isopropyl-4-methoxy-4-methylbicycl

Inchi: InChI=1S/C11H20O/c1-8(2)11-6-5-10(3,12-4)9(11)7-11/h8-9H,5-7H2,1-4H3
InchiKey: SCWGDYORLGVQND-UHFFFAOYSA-N
Formula: C11H20O
SMILES: COC1(C)CCC2(C(C)C)CC12
Mol. weight [g/mol]: 168.28
CAS: 1100111-06-5

Physical Properties

Property code	Value	Unit	Source
gf	37.11	kJ/mol	Joback Method
hf	-252.13	kJ/mol	Joback Method
hfus	6.66	kJ/mol	Joback Method
hvap	39.32	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.848		Crippen Method
mcvol	150.000	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	1120.20		NIST Webbook
rinpol	1120.20		NIST Webbook
tb	482.35	K	Joback Method
tc	689.43	K	Joback Method
tf	300.40	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.08	J/mol×K	482.35	Joback Method
cpg	381.32	J/mol×K	516.86	Joback Method
cpg	399.07	J/mol×K	551.38	Joback Method
cpg	415.52	J/mol×K	585.89	Joback Method
cpg	430.88	J/mol×K	620.40	Joback Method
cpg	445.36	J/mol×K	654.92	Joback Method
cpg	459.17	J/mol×K	689.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1100111065&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