3-((1R,2S,4S)-2-Methyl-3-methylenebicyclo[2.2.1]h

Inchi: InChI=1S/C12H18O/c1-9-10-4-5-11(8-10)12(9,2)6-3-7-13/h7,10-11H,1,3-6,8H2,2H3
InchiKey: LWTMDKBJLLLBBC-UHFFFAOYSA-N
Formula: C12H18O
SMILES: C=C1C2CCC(C2)C1(C)CCC=O
Mol. weight [g/mol]: 178.27
CAS: 26927-59-3

Physical Properties

Property code	Value	Unit	Source
gf	99.92	kJ/mol	Joback Method
hf	-158.01	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	47.72	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.958		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	1384.60		NIST Webbook
tb	535.10	K	Joback Method
tc	741.51	K	Joback Method
tf	332.70	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.40	J/mol×K	535.10	Joback Method
cpg	408.75	J/mol×K	569.50	Joback Method
cpg	424.97	J/mol×K	603.90	Joback Method
cpg	440.18	J/mol×K	638.31	Joback Method
cpg	454.52	J/mol×K	672.71	Joback Method
cpg	468.11	J/mol×K	707.11	Joback Method
cpg	481.10	J/mol×K	741.51	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=C26927593&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