santalone

Other names: 1-(2,3-Dimethyltricyclo[2.2.1.02,6]heptan-3-yl)ethanone
Inchi: InChI=1S/C11H16O/c1-6(12)10(2)7-4-8-9(5-7)11(8,10)3/h7-9H,4-5H2,1-3H3
InchiKey: OTAKYGLQNSNZRX-UHFFFAOYSA-N
Formula: C11H16O
SMILES: CC(=O)C1(C)C2CC3C(C2)C31C
Mol. weight [g/mol]: 164.24
CAS: 59300-51-5

Physical Properties

Property code	Value	Unit	Source
gf	92.87	kJ/mol	Joback Method
hf	-162.43	kJ/mol	Joback Method
hfus	14.00	kJ/mol	Joback Method
hvap	43.30	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.258		Crippen Method
mcvol	134.840	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1186.60		NIST Webbook
rinpol	1181.00		NIST Webbook
tb	507.77	K	Joback Method
tc	722.18	K	Joback Method
tf	363.84	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.47	J/mol×K	507.77	Joback Method
cpg	364.61	J/mol×K	543.51	Joback Method
cpg	380.17	J/mol×K	579.24	Joback Method
cpg	394.41	J/mol×K	614.98	Joback Method
cpg	407.63	J/mol×K	650.71	Joback Method
cpg	420.09	J/mol×K	686.45	Joback Method

cpg	432.06	J/mol×K	722.18	Joback Method

Sources

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=C59300515&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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