Acorenone

Inchi: InChI=1S/C15H24O/c1-10(2)13-6-5-12(4)15(13)8-7-11(3)14(16)9-15/h7,10,12-13H,5-6,8
InchiKey: HBTHUBMUAHAWBC-UMVBOHGHSA-N
Formula: C15H24O
SMILES: CC1=CCC2(CC1=O)C(C)CCC2C(C)C
Mol. weight [g/mol]: 220.35
CAS: 5956-05-8

Physical Properties

Property code	Value	Unit	Source
gf	30.62	kJ/mol	Joback Method
hf	-333.74	kJ/mol	Joback Method
hfus	14.07	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.984		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	1661.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1693.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	1988.00		NIST Webbook

tb	640.25	K	Joback Method
tc	873.95	K	Joback Method
tf	366.77	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.37	J/mol×K	640.25	Joback Method
cpg	586.37	J/mol×K	679.20	Joback Method
cpg	608.08	J/mol×K	718.15	Joback Method
cpg	628.63	J/mol×K	757.10	Joback Method
cpg	648.16	J/mol×K	796.05	Joback Method
cpg	666.81	J/mol×K	835.00	Joback Method
cpg	684.70	J/mol×K	873.95	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5956058&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

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