Acorenone B

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-SSDMNJCBSA-N
Formula: C15H24O
SMILES: CC1=CCC2(CC1=O)C(C)CCC2C(C)C
Mol. weight [g/mol]: 220.35
CAS: 21653-33-8

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	1696.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1701.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1676.00		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

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=C21653338&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