

(-)-nootkatone

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C15H24O/c1-10(2)12-5-6-13-8-14(16)7-11(3)15(13,4)9-12/h8,10-12H,5-7,9H2,
GQHRRBIPGXYEFT-SLEUVZQESA-N
C15H24O
CC(C)C1CCC2=CC(=O)CC(C)C2(C)C1
220.35
38427-78-0

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	1814.00		NIST Webbook
ripol	2515.00		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

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=C38427780&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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