

(E)-Nuciferal

Inchi:	InChI=1S/C15H20O/c1-13-8-10-15(11-9-13)7-5-3-4-6-14(2)12-16/h6,8-12H,3-5,7H2,1-2H
InchiKey:	IZFSDKNXOMAAQL-MKMNVTDBSA-N
Formula:	C15H20O
SMILES:	CC(C=O)=CCCCc1ccc(C)cc1
Mol. weight [g/mol]:	216.32

Physical Properties

Property code	Value	Unit	Source
gf	150.35	kJ/mol	Joback Method
hf	-106.02	kJ/mol	Joback Method
hfus	29.44	kJ/mol	Joback Method
hvap	58.68	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.853		Crippen Method
mcvol	195.720	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1701.00		NIST Webbook
rinpol	1701.00		NIST Webbook
tb	626.96	K	Joback Method
tc	833.85	K	Joback Method
tf	320.71	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.30	J/molxK	626.96	Joback Method
cpg	513.72	J/molxK	661.44	Joback Method
cpg	529.17	J/molxK	695.92	Joback Method
cpg	543.70	J/molxK	730.41	Joback Method
cpg	557.36	J/molxK	764.89	Joback Method
cpg	570.20	J/molxK	799.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232832&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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

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