

(Z)-Nuciferol isobutyrate

Inchi:	InChI=1S/C19H28O2/c1-14(2)19(20)21-13-16(4)7-6-8-17(5)18-11-9-15(3)10-12-18/h7,9-
InchiKey:	KGLMNOPKEMTZSH-APSNUPSMSA-N
Formula:	C19H28O2
SMILES:	CC(=CCCC(C)c1ccc(C)cc1)COC(=O)C(C)C
Mol. weight [g/mol]:	288.42

Physical Properties

Property code	Value	Unit	Source
gf	44.75	kJ/mol	Joback Method
hf	-358.36	kJ/mol	Joback Method
hfus	33.25	kJ/mol	Joback Method
hvap	69.24	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	5.024		Crippen Method
mvol	257.950	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	1997.00		NIST Webbook
tb	745.23	K	Joback Method
tc	950.80	K	Joback Method
tf	365.95	K	Joback Method
vc	0.985	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.67	J/mol×K	745.23	Joback Method
cpg	762.87	J/mol×K	779.49	Joback Method
cpg	779.97	J/mol×K	813.75	Joback Method
cpg	796.01	J/mol×K	848.02	Joback Method
cpg	811.05	J/mol×K	882.28	Joback Method
cpg	825.14	J/mol×K	916.54	Joback Method
cpg	838.31	J/mol×K	950.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R633760&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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