(Z)-Nuciferol

Inchi: InChI=1S/C15H22O/c1-13-8-10-15(11-9-13)7-5-3-4-6-14(2)12-16/h6,8-11,16H,3-5,7,12H
InchiKey: NAYBZOUJGHGOLI-NSIKDUERSA-N
Formula: C15H22O
SMILES: CC(=CCCCCc1ccc(C)cc1)CO
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	113.05	kJ/mol	Joback Method
hf	-172.67	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	68.64	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.646		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	1747.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1700.00		NIST Webbook
ripol	2545.00		NIST Webbook
ripol	2477.00		NIST Webbook
ripol	2477.00		NIST Webbook
tb	670.48	K	Joback Method
tc	862.99	K	Joback Method
tf	339.53	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	538.42	J/mol×K	670.48	Joback Method
cpg	553.40	J/mol×K	702.57	Joback Method
cpg	567.56	J/mol×K	734.65	Joback Method
cpg	580.95	J/mol×K	766.74	Joback Method
cpg	593.63	J/mol×K	798.82	Joback Method
cpg	605.62	J/mol×K	830.91	Joback Method
cpg	616.98	J/mol×K	862.99	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=R232872&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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