

6-(p-Tolyl)-2-methyl-2-heptenol, trans-

Other names:

(.+/-)-trans-Nuciferol
2-Hepten-1-ol, 2-methyl-6-(4-methylphenyl)-, (E)-(+/-)-
(.+/-)-(E)-Nuciferol
(2E)-2-Methyl-6-(4-methylphenyl)-2-hepten-1-ol
trans-Nuciferol
(E)-Nuciferol
Nuciferol (E)
Nuciferol

Inchi:

InChI=1S/C15H22O/c1-12-7-9-15(10-8-12)14(3)6-4-5-13(2)11-16/h5,7-10,14,16H,4,6,11

InchiKey:

FXCIQPDJVYFUQG-WLRTZDKTSA-N

Formula:

C15H22O

SMILES:

CC(=CCCC(C)c1ccc(C)cc1)CO

Mol. weight [g/mol]:

218.33

CAS:

39599-18-3

Physical Properties

Property code	Value	Unit	Source
gf	110.61	kJ/mol	Joback Method
hf	-177.95	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	68.25	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.817		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
tb	670.04	K	Joback Method
tc	865.73	K	Joback Method
tf	324.53	K	Joback Method
vc	0.761	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.91	J/mol×K	670.04	Joback Method

cpg	554.16	J/mol×K	702.66	Joback Method
cpg	568.57	J/mol×K	735.27	Joback Method
cpg	582.17	J/mol×K	767.89	Joback Method
cpg	595.02	J/mol×K	800.50	Joback Method
cpg	607.16	J/mol×K	833.12	Joback Method
cpg	618.65	J/mol×K	865.73	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=C39599183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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