(S,Z)-2-Methyl-6-(p-tolyl)hept-2-en-1-ol

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,4,6,11H
InchiKey: FXCIQPDJVYFUQG-MECSIWFOSA-N
Formula: C15H22O
SMILES: CC(=CCCC(C)c1ccc(C)cc1)CO
Mol. weight [g/mol]: 218.33
CAS: 78339-53-4

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
rinpol	1734.80		NIST Webbook
rinpol	1724.00		NIST Webbook
rinpol	1736.00		NIST Webbook
tb	670.04	K	Joback Method
tc	865.73	K	Joback Method
tf	324.53	K	Joback Method
vc	0.761	m3/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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78339534&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mcvol:	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