4-(Octylphenyl-3,6-dimethyl-1-cyclohexenyl ether

Inchi: InChI=1S/C22H34O/c1-4-5-6-7-8-9-10-20-13-15-21(16-14-20)23-22-17-18(2)11-12-19(22

InchiKey: TZNILEPZUINWMZ-UHFFFAOYSA-N

Formula: C22H34O

SMILES: CCCCCCCCc1ccc(OC2=CC(C)CCC2C)cc1

Mol. weight [g/mol]: 314.50

Physical Properties

Property code	Value	Unit	Source
gf	169.21	kJ/mol	Joback Method
hf	-324.28	kJ/mol	Joback Method
hfus	41.31	kJ/mol	Joback Method
hvap	70.99	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	6.918		Crippen Method
mcvol	287.790	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
ripol	3107.00		NIST Webbook
tb	775.86	K	Joback Method
tc	981.73	K	Joback Method
tf	415.29	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.15	J/mol×K	775.86	Joback Method
cpg	913.67	J/mol×K	810.17	Joback Method
cpg	933.80	J/mol×K	844.48	Joback Method
cpg	952.58	J/mol×K	878.79	Joback Method
cpg	970.04	J/mol×K	913.10	Joback Method
cpg	986.23	J/mol×K	947.41	Joback Method
cpg	1001.19	J/mol×K	981.73	Joback Method
dvisc	0.0009883	Pa×s	415.29	Joback Method
dvisc	0.0005035	Pa×s	475.38	Joback Method

dvisc	0.0002984	Pa×s	535.48	Joback Method
dvisc	0.0001966	Pa×s	595.58	Joback Method
dvisc	0.0001398	Pa×s	655.67	Joback Method
dvisc	0.0001052	Pa×s	715.77	Joback Method
dvisc	0.0000828	Pa×s	775.86	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R58561&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
dvisc: Dynamic viscosity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume