4-Sec-butyl-2,6-dicyclohexylphenol

Inchi: InChI=1S/C22H34O/c1-3-16(2)19-14-20(17-10-6-4-7-11-17)22(23)21(15-19)18-12-8-5-9-
InchiKey: IUPNCOGRTZRLMM-UHFFFAOYSA-N
Formula: C22H34O
SMILES: CCC(C)c1cc(C2CCCCC2)c(O)c(C2CCCCC2)c1
Mol. weight [g/mol]: 314.50
CAS: 52938-79-1

Physical Properties

Property code	Value	Unit	Source
gf	119.35	kJ/mol	Joback Method
hf	-357.77	kJ/mol	Joback Method
hfus	31.93	kJ/mol	Joback Method
hvap	81.65	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	7.001		Crippen Method
mcvol	281.230	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
tb	858.68	K	Joback Method
tc	1103.71	K	Joback Method
tf	500.64	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.81	J/mol×K	858.68	Joback Method
cpg	1049.90	J/mol×K	1062.87	Joback Method
cpg	1032.61	J/mol×K	1022.03	Joback Method
cpg	1014.21	J/mol×K	981.19	Joback Method
cpg	994.55	J/mol×K	940.36	Joback Method
cpg	973.46	J/mol×K	899.52	Joback Method
cpg	1066.24	J/mol×K	1103.71	Joback Method
dvisc	0.0000037	Pa×s	858.68	Joback Method
dvisc	0.0000058	Pa×s	799.01	Joback Method

dvisc	0.0000098	Pa×s	739.33	Joback Method
dvisc	0.0000180	Pa×s	679.66	Joback Method
dvisc	0.0000370	Pa×s	619.99	Joback Method
dvisc	0.0000891	Pa×s	560.31	Joback Method
dvisc	0.0002644	Pa×s	500.64	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=C52938791&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume