Curcuphenol

Inchi: InChI=1S/C15H22O/c1-11(2)6-5-7-13(4)14-9-8-12(3)10-15(14)16/h6,8-10,13,16H,5,7H2,
InchiKey: BTXSROVNGICYFE-UHFFFAOYSA-N
Formula: C15H22O
SMILES: CC(C)=CCCC(C)c1ccc(C)cc1O
Mol. weight [g/mol]: 218.33
CAS: 69301-27-5

Physical Properties

Property code	Value	Unit	Source
gf	92.81	kJ/mol	Joback Method
hf	-203.03	kJ/mol	Joback Method
hfus	29.41	kJ/mol	Joback Method
hvap	64.59	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.551		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1719.00		NIST Webbook
rinpol	1697.00		NIST Webbook
rinpol	1722.70		NIST Webbook
rinpol	1694.00		NIST Webbook
tb	658.48	K	Joback Method
tc	876.37	K	Joback Method
tf	375.43	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.73	J/mol×K	658.48	Joback Method
cpg	552.43	J/mol×K	694.79	Joback Method
cpg	568.15	J/mol×K	731.11	Joback Method
cpg	582.99	J/mol×K	767.42	Joback Method
cpg	597.04	J/mol×K	803.74	Joback Method

cpg	610.41	J/mol×K	840.05	Joback Method
cpg	623.20	J/mol×K	876.37	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=C69301275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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