

2-(4-Methylphenyl)-2-(4-hydroxyphenyl)propane

Inchi: InChI=1S/C16H18O/c1-12-4-6-13(7-5-12)16(2,3)14-8-10-15(17)11-9-14/h4-11,17H,1-3H3
InchiKey: SZQFXKGNLRDAND-UHFFFAOYSA-N
Formula: C16H18O
SMILES: Cc1ccc(C(C)(C)c2ccc(O)cc2)cc1
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	147.25	kJ/mol	Joback Method
hf	-98.04	kJ/mol	Joback Method
hfus	23.26	kJ/mol	Joback Method
hvap	68.14	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	4.027		Crippen Method
mcvol	194.650	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	1961.00		NIST Webbook
tb	701.21	K	Joback Method
tc	954.53	K	Joback Method
tf	449.58	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.18	J/mol×K	701.21	Joback Method
cpg	603.66	J/mol×K	912.31	Joback Method
cpg	590.95	J/mol×K	870.09	Joback Method
cpg	577.54	J/mol×K	827.87	Joback Method
cpg	563.23	J/mol×K	785.65	Joback Method
cpg	547.84	J/mol×K	743.43	Joback Method
cpg	615.84	J/mol×K	954.53	Joback Method
dvisc	0.0000115	Pa×s	701.21	Joback Method
dvisc	0.0000175	Pa×s	659.27	Joback Method

dvisc	0.0000280	Pa×s	617.33	Joback Method
dvisc	0.0000481	Pa×s	575.39	Joback Method
dvisc	0.0000900	Pa×s	533.46	Joback Method
dvisc	0.0001875	Pa×s	491.52	Joback Method
dvisc	0.0004476	Pa×s	449.58	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=R569010&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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