

2-Methyl-6-(1-phenylbutyl)phenol

Inchi:	InChI=1S/C17H20O/c1-3-8-15(14-10-5-4-6-11-14)16-12-7-9-13(2)17(16)18/h4-7,9-12,15
InchiKey:	IDWTUXABKUCYJN-UHFFFAOYSA-N
Formula:	C17H20O
SMILES:	CCCC(c1ccccc1)c1cccc(C)c1O
Mol. weight [g/mol]:	240.34

Physical Properties

Property code	Value	Unit	Source
gf	150.39	kJ/mol	Joback Method
hf	-115.21	kJ/mol	Joback Method
hfus	29.74	kJ/mol	Joback Method
hvap	71.28	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.633		Crippen Method
mcvol	208.740	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	1856.00		NIST Webbook
rinpol	1856.00		NIST Webbook
tb	726.88	K	Joback Method
tc	965.77	K	Joback Method
tf	443.43	K	Joback Method
vc	0.732	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.34	J/molxK	726.88	Joback Method
cpg	599.10	J/molxK	766.69	Joback Method
cpg	614.75	J/molxK	806.51	Joback Method
cpg	629.42	J/molxK	846.32	Joback Method
cpg	643.23	J/molxK	886.14	Joback Method
cpg	656.33	J/molxK	925.95	Joback Method
cpg	668.85	J/molxK	965.77	Joback Method
dvisc	0.0005241	Paxs	443.43	Joback Method

dvisc	0.0001982	Paxs	490.67	Joback Method
dvisc	0.0000890	Paxs	537.91	Joback Method
dvisc	0.0000454	Paxs	585.15	Joback Method
dvisc	0.0000257	Paxs	632.40	Joback Method
dvisc	0.0000157	Paxs	679.64	Joback Method
dvisc	0.0000102	Paxs	726.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R590613&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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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