

4-(4-hydroxy-3-methoxyphenyl)-1-butanol

Inchi:	InChI=1S/C11H16O3/c1-14-11-8-9(4-2-3-7-12)5-6-10(11)13/h5-6,8,12-13H,2-4,7H2,1H3
InchiKey:	KYIMBEHWPPBVMU-UHFFFAOYSA-N
Formula:	C11H16O3
SMILES:	COc1cc(CCCCO)ccc1O
Mol. weight [g/mol]:	196.24

Physical Properties

Property code	Value	Unit	Source
gf	-251.92	kJ/mol	Joback Method
hf	-507.07	kJ/mol	Joback Method
hfus	28.96	kJ/mol	Joback Method
hvap	75.12	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.716		Crippen Method
mvol	159.700	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
ripol	2865.00		NIST Webbook
ripol	2865.00		NIST Webbook
tb	677.96	K	Joback Method
tc	877.57	K	Joback Method
tf	447.44	K	Joback Method
vc	0.546	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.92	J/molxK	677.96	Joback Method
cpg	485.78	J/molxK	844.31	Joback Method
cpg	476.42	J/molxK	811.04	Joback Method
cpg	466.60	J/molxK	777.77	Joback Method
cpg	456.28	J/molxK	744.50	Joback Method
cpg	445.40	J/molxK	711.23	Joback Method
cpg	494.73	J/molxK	877.57	Joback Method
dvisc	0.0000051	Paxs	677.96	Joback Method

dvisc	0.0000085	Paxs	639.54	Joback Method
dvisc	0.0000149	Paxs	601.12	Joback Method
dvisc	0.0000285	Paxs	562.70	Joback Method
dvisc	0.0000597	Paxs	524.28	Joback Method
dvisc	0.0001408	Paxs	485.86	Joback Method
dvisc	0.0003844	Paxs	447.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R317745&Units=SI

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

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