2-(.alpha.,.alpha.-dimethylbenzyl) phenol

Other names: o-(«alpha»,«alpha»-Dimethylbenzyl)phenol
2-(«alpha»,«alpha»-Dimethylbenzyl)phenol
Dimethylphenol-2-ylphenylmethane
Inchi: InChI=1S/C15H16O/c1-15(2,12-8-4-3-5-9-12)13-10-6-7-11-14(13)16/h3-11,16H,1-2H3
InchiKey: CJWNFAKWHDOUKL-UHFFFAOYSA-N
Formula: C15H16O
SMILES: CC(C)(c1ccccc1)c1ccccc1O
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
af	0.5588		Cheméo Relay (1.0)
hf	-35.78	kJ/mol	Cheméo Relay (1.0)
hfus	21.06	kJ/mol	Joback Method
hvap	90.87	kJ/mol	Cheméo Relay (1.0)
ie	7.96	eV	Cheméo Relay (1.0)
log10ws	-3.46		Cheméo Relay (1.0)
logp	3.718		Crippen Method
mcvol	180.560	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	570.16	K	Cheméo Relay (1.0)
tc	855.48	K	Cheméo Relay (1.0)
tf	326.35	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.34	J/mol×K	673.35	Joback Method
cpg	562.39	J/mol×K	931.82	Joback Method
cpg	550.83	J/mol×K	888.74	Joback Method
cpg	538.68	J/mol×K	845.66	Joback Method
cpg	525.77	J/mol×K	802.58	Joback Method
cpg	511.88	J/mol×K	759.51	Joback Method
cpg	496.80	J/mol×K	716.43	Joback Method

dvisc	0.0000674	Pa×s	549.57	Joback Method
dvisc	0.0000148	Pa×s	673.35	Joback Method
dvisc	0.0000229	Pa×s	632.09	Joback Method
dvisc	0.0000379	Pa×s	590.83	Joback Method
dvisc	0.0007455	Pa×s	425.79	Joback Method
dvisc	0.0001319	Pa×s	508.31	Joback Method
dvisc	0.0002905	Pa×s	467.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18168406&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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