Phenol, o-(«alpha»,«alpha»-dimethylbenzyl)-

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
CAS:	18168-40-6

Physical Properties

Property code	Value	Unit	Source
gf	148.46	kJ/mol	Joback Method
hf	-65.93	kJ/mol	Joback Method
hfus	21.06	kJ/mol	Joback Method
hvap	65.25	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.718		Crippen Method
mcvol	180.560	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	673.35	K	Joback Method
tc	931.82	K	Joback Method
tf	425.79	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

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

cpg	562.39	J/mol×K	931.82	Joback Method
dvisc	0.0007455	Pa×s	425.79	Joback Method
dvisc	0.0002905	Pa×s	467.05	Joback Method
dvisc	0.0001319	Pa×s	508.31	Joback Method
dvisc	0.0000674	Pa×s	549.57	Joback Method
dvisc	0.0000379	Pa×s	590.83	Joback Method
dvisc	0.0000229	Pa×s	632.09	Joback Method
dvisc	0.0000148	Pa×s	673.35	Joback Method

Sources

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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume