4-sec-Butyl-2-(«alpha»-methylbenzyl)phenol

Other names:	4-sec-Butyl-2-(«alpha»-methylbenzyl)alcohol
	Phenol, 4-(1-methylpropyl)-2-(1-phenylethyl)-
	Phenol, 4-sec-butyl-2-(«alpha»-methylbenzyl)-
	4-(1-methylpropyl)-2-(1-phenylethyl)phenol
	4-Sec-butyl-2-(a-methylbenzyl)phenol
Inchi:	InChI=1S/C18H22O/c1-4-13(2)16-10-11-18(19)17(12-16)14(3)15-8-6-5-7-9-15/h5-14,19H
InchiKey:	QJNBIFRUSFIANU-UHFFFAOYSA-N
Formula:	C18H22O
SMILES:	CCC(C)c1ccc(O)c(C(C)c2ccccc2)c1
Mol. weight [g/mol]:	254.37
CAS:	2622-83-5

Physical Properties

Property code	Value	Unit	Source
gf	156.37	kJ/mol	Joback Method
hf	-141.13	kJ/mol	Joback Method
hfus	28.81	kJ/mol	Joback Method
hvap	73.11	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	5.058		Crippen Method
mcvol	222.830	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
tb	749.32	K	Joback Method
tc	988.04	K	Joback Method
tf	439.70	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.42	J/mol×K	749.32	Joback Method
cpg	714.44	J/mol×K	948.26	Joback Method
cpg	700.76	J/mol×K	908.47	Joback Method
cpg	686.35	J/mol×K	868.68	Joback Method

cpg	671.09	J/mol×K	828.89	Joback Method
cpg	654.82	J/mol×K	789.11	Joback Method
cpg	727.53	J/mol×K	988.04	Joback Method
dvisc	0.0000077	Pa×s	749.32	Joback Method
dvisc	0.0000121	Pa×s	697.72	Joback Method
dvisc	0.0000205	Pa×s	646.11	Joback Method
dvisc	0.0000381	Pa×s	594.51	Joback Method
dvisc	0.0000797	Pa×s	542.91	Joback Method
dvisc	0.0001944	Pa×s	491.30	Joback Method
dvisc	0.0005848	Pa×s	439.70	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	450.00 ± 3.00	K	0.30	NIST Webbook

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=C2622835&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume