2-(«alpha»-Methylbenzyl)-p-cresol

Inchi: InChI=1S/C15H16O/c1-11-8-9-15(16)14(10-11)12(2)13-6-4-3-5-7-13/h3-10,12,16H,1-2H
InchiKey: DJRYJQNZAYJVGF-UHFFFAOYSA-N
Formula: C15H16O
SMILES: Cc1ccc(O)c(C(C)c2ccccc2)c1
Mol. weight [g/mol]: 212.29
CAS: 1817-67-0

Physical Properties

Property code	Value	Unit	Source
gf	133.55	kJ/mol	Joback Method
hf	-73.93	kJ/mol	Joback Method
hfus	24.56	kJ/mol	Joback Method
hvap	66.82	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.852		Crippen Method
mcvol	180.560	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1766.60		NIST Webbook
tb	681.12	K	Joback Method
tc	930.41	K	Joback Method
tf	420.89	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.89	J/mol×K	681.12	Joback Method
cpg	492.85	J/mol×K	722.67	Joback Method
cpg	507.63	J/mol×K	764.22	Joback Method
cpg	521.38	J/mol×K	805.76	Joback Method
cpg	534.23	J/mol×K	847.31	Joback Method
cpg	546.33	J/mol×K	888.86	Joback Method
cpg	557.81	J/mol×K	930.41	Joback Method
dvisc	0.0007566	Pa×s	420.89	Joback Method

dvisc	0.0002920	Pa×s	464.26	Joback Method
dvisc	0.0001326	Pa×s	507.63	Joback Method
dvisc	0.0000682	Pa×s	551.01	Joback Method
dvisc	0.0000386	Pa×s	594.38	Joback Method
dvisc	0.0000237	Pa×s	637.75	Joback Method
dvisc	0.0000154	Pa×s	681.12	Joback Method

Sources

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=C1817670&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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