4-n-Dodecylresorcinol

Other names:	4-n-Laurylresorcinol
	1,3-Benzenediol, 4-dodecyl-
	4-dodecylresorcinol
Inchi:	InChI=1S/C18H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-16-13-14-17(19)15-18(16)20/h13-15,1
InchiKey:	JJWVPHWHEGQZOE-UHFFFAOYSA-N
Formula:	C18H30O2
SMILES:	CCCCCCCCCCCCc1ccc(O)cc1O
Mol. weight [g/mol]:	278.43
CAS:	24305-56-4

Physical Properties

Property code	Value	Unit	Source
gf	-96.15	kJ/mol	Joback Method
hf	-532.94	kJ/mol	Joback Method
hfus	47.98	kJ/mol	Joback Method
hvap	83.97	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.561		Crippen Method
mcvol	252.460	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
tb	799.16	K	Joback Method
tc	1004.25	K	Joback Method
tf	542.48	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.38	J/mol×K	799.16	Joback Method
cpg	799.97	J/mol×K	833.34	Joback Method
cpg	815.95	J/mol×K	867.52	Joback Method
cpg	831.44	J/mol×K	901.70	Joback Method
cpg	846.55	J/mol×K	935.88	Joback Method
cpg	861.39	J/mol×K	970.06	Joback Method

cpg	876.10	J/mol×K	1004.25	Joback Method
dvisc	0.0000288	Pa×s	542.48	Joback Method
dvisc	0.0000111	Pa×s	585.26	Joback Method
dvisc	0.0000049	Pa×s	628.04	Joback Method
dvisc	0.0000024	Pa×s	670.82	Joback Method
dvisc	0.0000013	Pa×s	713.60	Joback Method
dvisc	0.0000007	Pa×s	756.38	Joback Method
dvisc	0.0000004	Pa×s	799.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	498.20	K	0.80	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24305564&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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