4-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]: 278.44

Physical Properties

Property code	Value	Unit	Source
hfus	47.98	kJ/mol	Joback Method
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-5.95		Cheméo Relay (1.0)
logp	5.561		Crippen Method
mcvol	252.460	ml/mol	McGowan Method
tb	627.80	K	Cheméo Relay (1.0)
tf	369.55	K	Cheméo Relay (1.0)

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
Joback Method: https://en.wikipedia.org/wiki/Joback_method
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):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point