3-Tridecylphenol

Inchi: InChI=1S/C19H32O/c1-2-3-4-5-6-7-8-9-10-11-12-14-18-15-13-16-19(20)17-18/h13,15-17

InchiKey: IFGRPNIAGKTMCH-UHFFFAOYSA-N

Formula: C19H32O

SMILES: CCCCCCCCCCCCCc1cccc(O)c1

Mol. weight [g/mol]:   276.46

CAS: 72424-02-3

Physical Properties

Property code	Value	Unit	Source
gf	66.89	kJ/mol	Joback Method
hf	-376.27	kJ/mol	Joback Method
hfus	44.79	kJ/mol	Joback Method
hvap	73.18	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	6.246		Crippen Method
mcvol	260.680	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2286.10		NIST Webbook
rinpol	2294.00		NIST Webbook
tb	741.42	K	Joback Method
tc	935.65	K	Joback Method
tf	442.03	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.07	J/mol×K	741.42	Joback Method
cpg	797.27	J/mol×K	773.79	Joback Method
cpg	814.56	J/mol×K	806.16	Joback Method
cpg	831.02	J/mol×K	838.54	Joback Method
cpg	846.74	J/mol×K	870.91	Joback Method
cpg	861.78	J/mol×K	903.28	Joback Method
cpg	876.22	J/mol×K	935.65	Joback Method

dvisc	0.0005671	Pa×s	442.03	Joback Method
dvisc	0.0001953	Pa×s	491.93	Joback Method
dvisc	0.0000818	Pa×s	541.83	Joback Method
dvisc	0.0000397	Pa×s	591.73	Joback Method
dvisc	0.0000216	Pa×s	641.62	Joback Method
dvisc	0.0000128	Pa×s	691.52	Joback Method
dvisc	0.0000081	Pa×s	741.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72424023&Units=SI

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