

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:	CCCCCCCCCCCCCc1ccc(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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72424023&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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