Phenol, 2-octyl-

Other names: Phenol, o-octyl-
o-Octylphenol
2-Octylphenol
Inchi: InChI=1S/C14H22O/c1-2-3-4-5-6-7-10-13-11-8-9-12-14(13)15/h8-9,11-12,15H,2-7,10H2,
InchiKey: DUIOKRXOKLLURE-UHFFFAOYSA-N
Formula: C14H22O
SMILES: CCCCCCCCc1ccccc1O
Mol. weight [g/mol]: 206.32
CAS: 949-13-3

Physical Properties

Property code	Value	Unit	Source
gf	24.79	kJ/mol	Joback Method
hf	-273.07	kJ/mol	Joback Method
hfus	31.84	kJ/mol	Joback Method
hvap	62.05	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.295		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
ripol	2282.00		NIST Webbook
ripol	2282.00		NIST Webbook
tb	627.02	K	Joback Method
tc	831.64	K	Joback Method
tf	385.68	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.42	J/mol×K	627.02	Joback Method
cpg	578.57	J/mol×K	797.54	Joback Method
cpg	565.52	J/mol×K	763.43	Joback Method
cpg	551.75	J/mol×K	729.33	Joback Method

cpg	537.19	J/mol×K	695.23	Joback Method
cpg	521.77	J/mol×K	661.12	Joback Method
cpg	590.99	J/mol×K	831.64	Joback Method
dvisc	0.0000243	Pa×s	627.02	Joback Method
dvisc	0.0000384	Pa×s	586.80	Joback Method
dvisc	0.0000648	Pa×s	546.57	Joback Method
dvisc	0.0001189	Pa×s	506.35	Joback Method
dvisc	0.0002421	Pa×s	466.13	Joback Method
dvisc	0.0005642	Pa×s	425.90	Joback Method
dvisc	0.0015682	Pa×s	385.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C949133&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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