2,5-Diethylphenol

Inchi:	InChI=1S/C10H14O/c1-3-8-5-6-9(4-2)10(11)7-8/h5-7,11H,3-4H2,1-2H3
InchiKey:	AQFCDVGUEQOTAC-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CCc1ccc(CC)c(O)c1
Mol. weight [g/mol]:	150.22
CAS:	876-20-0

Physical Properties

Property code	Value	Unit	Source
gf	-18.52	kJ/mol	Joback Method
hf	-201.98	kJ/mol	Joback Method
hfus	21.09	kJ/mol	Joback Method
hvap	53.81	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.517		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
rinpol	1271.00		NIST Webbook
rinpol	1271.00		NIST Webbook
ripol	1987.00		NIST Webbook
ripol	1987.00		NIST Webbook
ripol	1987.00		NIST Webbook
tb	540.48	K	Joback Method
tc	759.98	K	Joback Method
tf	353.12	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.31	J/mol×K	540.48	Joback Method
cpg	324.79	J/mol×K	577.06	Joback Method
cpg	337.41	J/mol×K	613.65	Joback Method
cpg	349.24	J/mol×K	650.23	Joback Method

cpg	360.34	J/mol×K	686.81	Joback Method
cpg	370.79	J/mol×K	723.39	Joback Method
cpg	380.67	J/mol×K	759.98	Joback Method
dvisc	0.0022455	Pa×s	353.12	Joback Method
dvisc	0.0009482	Pa×s	384.35	Joback Method
dvisc	0.0004558	Pa×s	415.57	Joback Method
dvisc	0.0002427	Pa×s	446.80	Joback Method
dvisc	0.0001403	Pa×s	478.03	Joback Method
dvisc	0.0000868	Pa×s	509.25	Joback Method
dvisc	0.0000567	Pa×s	540.48	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46228e+01
Coeff. B	-4.29840e+03
Coeff. C	-8.01500e+01
Temperature range (K), min.	380.00
Temperature range (K), max.	541.78

Sources

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=C876200&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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