

3,4-Diethylphenol

Inchi:	InChI=1S/C10H14O/c1-3-8-5-6-10(11)7-9(8)4-2/h5-7,11H,3-4H2,1-2H3
InchiKey:	SEAZSNZFNABEMJ-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CCc1ccc(O)cc1CC
Mol. weight [g/mol]:	150.22
CAS:	875-85-4

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	1284.00		NIST Webbook
rinpol	1318.00		NIST Webbook
tb	540.48	K	Joback Method
tc	759.98	K	Joback Method
tf	353.12	K	Joback Method
vc	0.454	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.31	J/molxK	540.48	Joback Method
cpg	370.79	J/molxK	723.39	Joback Method
cpg	360.34	J/molxK	686.81	Joback Method
cpg	349.24	J/molxK	650.23	Joback Method
cpg	337.41	J/molxK	613.65	Joback Method
cpg	324.79	J/molxK	577.06	Joback Method
cpg	380.67	J/molxK	759.98	Joback Method

dvisc	0.0000567	Paxs	540.48	Joback Method
dvisc	0.0000868	Paxs	509.25	Joback Method
dvisc	0.0001403	Paxs	478.03	Joback Method
dvisc	0.0002427	Paxs	446.80	Joback Method
dvisc	0.0004558	Paxs	415.57	Joback Method
dvisc	0.0009482	Paxs	384.35	Joback Method
dvisc	0.0022455	Paxs	353.12	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54655e+01
Coeff. B	-4.63032e+03
Coeff. C	-8.29300e+01
Temperature range (K), min.	388.00
Temperature range (K), max.	538.94

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C875854&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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