Phenol, 4-(1,2-diethylpentyl)

Inchi: InChI=1S/C15H24O/c1-4-7-12(5-2)15(6-3)13-8-10-14(16)11-9-13/h8-12,15-16H,4-7H2,1-
InchiKey: HJALBPRTWBCBOD-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CCCC(CC)C(CC)c1ccc(O)cc1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hf	-268.78	kJ/mol	Cheméo Relay (1.0)
hfus	27.38	kJ/mol	Joback Method
hvap	87.05	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.71		Cheméo Relay (1.0)
logp	4.712		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
rinpol	1761.00		NIST Webbook
tb	582.97	K	Cheméo Relay (1.0)
tf	334.30	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-5.69360e+01
Coeff. B	1.51636e+00
Coeff. C	-1.08616e-03
Coeff. D	3.24900e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.76838e+01
Coeff. B	4.34468e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	366.95
Temperature range (K), max.	601.06

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R592535&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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