

(Z)-3-(pentadec-8-en-1-yl)phenol

Inchi:	InChI=1S/C21H34O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-16-20-17-15-18-21(22)19-20/h7-
InchiKey:	YLKVIMNNMLKUGJ-FPLPWBNLSA-N
Formula:	C21H34O
SMILES:	CCCCCCC=CCCCCCCCc1cccc(O)c1
Mol. weight [g/mol]:	302.49
CAS:	501-26-8

Physical Properties

Property code	Value	Unit	Source
gf	163.95	kJ/mol	Joback Method
hf	-300.33	kJ/mol	Joback Method
hfus	50.17	kJ/mol	Joback Method
hvap	77.59	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	6.802		Crippen Method
mcvol	284.560	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinpol	2479.00		NIST Webbook
rinpol	2479.00		NIST Webbook
tb	791.34	K	Joback Method
tc	989.42	K	Joback Method
tf	459.49	K	Joback Method
vc	1.050	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.60	J/molxK	791.34	Joback Method
cpg	890.02	J/molxK	824.35	Joback Method
cpg	907.59	J/molxK	857.37	Joback Method
cpg	924.41	J/molxK	890.38	Joback Method
cpg	940.56	J/molxK	923.39	Joback Method
cpg	956.16	J/molxK	956.41	Joback Method
cpg	971.29	J/molxK	989.42	Joback Method

dvisc	0.0003670	Paxs	459.49	Joback Method
dvisc	0.0001192	Paxs	514.80	Joback Method
dvisc	0.0000481	Paxs	570.11	Joback Method
dvisc	0.0000228	Paxs	625.42	Joback Method
dvisc	0.0000122	Paxs	680.72	Joback Method
dvisc	0.0000072	Paxs	736.03	Joback Method
dvisc	0.0000046	Paxs	791.34	Joback Method

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=C501268&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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