

2,4-Dinonylphenol

Inchi:	InChI=1S/C24H42O/c1-3-5-7-9-11-13-15-17-22-19-20-24(25)23(21-22)18-16-14-12-10-8
InchiKey:	FDAJTLLBHNHECW-UHFFFAOYSA-N
Formula:	C24H42O
SMILES:	CCCCCCCCc1ccc(O)c(CCCCCCCC)c1
Mol. weight [g/mol]:	346.59
CAS:	137-99-5

Physical Properties

Property code	Value	Unit	Source
gf	99.36	kJ/mol	Joback Method
hf	-490.94	kJ/mol	Joback Method
hfus	57.35	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	7.978		Crippen Method
mvol	331.130	ml/mol	McGowan Method
pc	1070.06	kPa	Joback Method
tb	860.80	K	Joback Method
tc	1058.59	K	Joback Method
tf	510.90	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.54	J/molxK	860.80	Joback Method
cpg	1171.51	J/molxK	1025.62	Joback Method
cpg	1154.54	J/molxK	992.66	Joback Method
cpg	1136.94	J/molxK	959.69	Joback Method
cpg	1118.63	J/molxK	926.73	Joback Method
cpg	1099.53	J/molxK	893.76	Joback Method
cpg	1187.94	J/molxK	1058.59	Joback Method
dvisc	0.0000028	Paxs	860.80	Joback Method
dvisc	0.0000043	Paxs	802.48	Joback Method

dvisc	0.0000071	Paxs	744.17	Joback Method
dvisc	0.0000127	Paxs	685.85	Joback Method
dvisc	0.0000252	Paxs	627.53	Joback Method
dvisc	0.0000576	Paxs	569.22	Joback Method
dvisc	0.0001592	Paxs	510.90	Joback Method

Sources

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=C137995&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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