

Phenol, 2-(1-methylpentyl)-4-nitro

Inchi:	InChI=1S/C12H17NO3/c1-3-4-5-9(2)11-8-10(13(15)16)6-7-12(11)14/h6-9,14H,3-5H2,1-2
InchiKey:	MIAILGMNACGFSB-UHFFFAOYSA-N
Formula:	C12H17NO3
SMILES:	CCCCC(C)c1cc([N+](=O)[O-])ccc1O
Mol. weight [g/mol]:	223.27

Physical Properties

Property code	Value	Unit	Source
gf	31.43	kJ/mol	Joback Method
hf	-259.30	kJ/mol	Joback Method
hfus	34.11	kJ/mol	Joback Method
hvap	74.46	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.594		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpola	1960.00		NIST Webbook
rinpola	1960.00		NIST Webbook
tb	737.64	K	Joback Method
tc	975.34	K	Joback Method
tf	504.27	K	Joback Method
vc	0.641	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.19	J/molxK	737.64	Joback Method
cpg	521.85	J/molxK	777.26	Joback Method
cpg	534.66	J/molxK	816.87	Joback Method
cpg	546.75	J/molxK	856.49	Joback Method
cpg	558.20	J/molxK	896.11	Joback Method
cpg	569.14	J/molxK	935.72	Joback Method
cpg	579.66	J/molxK	975.34	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=R58717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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