

# Fluoranthene, 1,7-dinitro

<b>Inchi:</b>	InChI=1S/C16H8N2O4/c19-17(20)12-6-2-5-11-15(12)10-4-1-3-9-7-8-13(18(21)22)16(11)
<b>InchiKey:</b>	DUESYCHFBLSMHF-UHFFFAOYSA-N
<b>Formula:</b>	C16H8N2O4
<b>SMILES:</b>	O=[N+]([O-])c1cccc2c1-c1cccc3ccc([N+](=O)[O-])c-2c13
<b>Mol. weight [g/mol]:</b>	292.25

## Physical Properties

Property code	Value	Unit	Source
gf	543.02	kJ/mol	Joback Method
hf	323.31	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	93.60	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	4.304		Crippen Method
mcvol	193.300	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	455.80		NIST Webbook
tb	965.00	K	Joback Method
tc	1252.37	K	Joback Method
tf	738.18	K	Joback Method
vc	0.783	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.72	J/molxK	965.00	Joback Method
cpg	565.01	J/molxK	1012.90	Joback Method
cpg	576.59	J/molxK	1060.79	Joback Method
cpg	588.77	J/molxK	1108.69	Joback Method
cpg	601.84	J/molxK	1156.58	Joback Method
cpg	616.09	J/molxK	1204.48	Joback Method
cpg	631.81	J/molxK	1252.37	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R36882&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R36882&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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