

# Fumaric acid, naphth-1-yl naphth-2-ylmethyl ester

Inchi:	InChI=1S/C25H18O4/c26-24(28-17-18-12-13-19-6-1-2-8-21(19)16-18)14-15-25(27)29-23
InchiKey:	CUVUNBQRAYTETL-CCEZHUSRSA-N
Formula:	C25H18O4
SMILES:	O=C(C=CC(=O)Oc1cccc2ccccc12)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	382.41

## Physical Properties

Property code	Value	Unit	Source
gf	190.86	kJ/mol	Joback Method
hf	-99.45	kJ/mol	Joback Method
hfus	47.62	kJ/mol	Joback Method
hvap	98.67	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	5.198		Crippen Method
mcvol	287.250	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	3351.00		NIST Webbook
rinpol	3351.00		NIST Webbook
tb	1029.42	K	Joback Method
tc	1285.93	K	Joback Method
tf	654.03	K	Joback Method
vc	1.091	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.94	J/molxK	1029.42	Joback Method
cpg	935.93	J/molxK	1243.18	Joback Method
cpg	924.91	J/molxK	1200.43	Joback Method
cpg	913.78	J/molxK	1157.68	Joback Method
cpg	902.35	J/molxK	1114.92	Joback Method
cpg	890.46	J/molxK	1072.17	Joback Method
cpg	947.00	J/molxK	1285.93	Joback Method
dvisc	0.0001118	Paxs	1029.42	Joback Method

dvisc	0.0001329	Paxs	966.86	Joback Method
dvisc	0.0001618	Paxs	904.29	Joback Method
dvisc	0.0002027	Paxs	841.73	Joback Method
dvisc	0.0002635	Paxs	779.16	Joback Method
dvisc	0.0003584	Paxs	716.60	Joback Method
dvisc	0.0005171	Paxs	654.03	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U405820&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405820&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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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