

# But-2-enamide, N,N-bis(2-ethylhexyl)-3-methyl-

**Inchi:** InChI=1S/C21H41NO/c1-7-11-13-19(9-3)16-22(21(23)15-18(5)6)17-20(10-4)14-12-8-2/h  
**InchiKey:** BEVUJVCVSUBJOK-UHFFFAOYSA-N  
**Formula:** C21H41NO  
**SMILES:** CCCCC(CC)CN(CC(CC)CCCC)C(=O)C=C(C)C  
**Mol. weight [g/mol]:** 323.56

## Physical Properties

Property code	Value	Unit	Source
gf	174.59	kJ/mol	Joback Method
hf	-424.95	kJ/mol	Joback Method
hfus	46.61	kJ/mol	Joback Method
hvap	70.39	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	6.214		Crippen Method
mcvol	314.000	ml/mol	McGowan Method
pc	1040.58	kPa	Joback Method
rinpol	2073.00		NIST Webbook
tb	749.35	K	Joback Method
tc	928.02	K	Joback Method
tf	359.79	K	Joback Method
vc	1.204	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.60	J/molxK	749.35	Joback Method
cpg	976.98	J/molxK	779.13	Joback Method
cpg	996.35	J/molxK	808.91	Joback Method
cpg	1014.76	J/molxK	838.68	Joback Method
cpg	1032.27	J/molxK	868.46	Joback Method
cpg	1048.91	J/molxK	898.24	Joback Method
cpg	1064.75	J/molxK	928.02	Joback Method

# Sources

<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=U308239&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308239&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

## 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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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