

But-2-enamide, N,N-dihexyl-3-methyl-

Inchi:	InChI=1S/C17H33NO/c1-5-7-9-11-13-18(14-12-10-8-6-2)17(19)15-16(3)4/h15H,5-14H2,1
InchiKey:	HLRCZNMMMYNCMC-UHFFFAOYSA-N
Formula:	C17H33NO
SMILES:	CCCCCN(CCCCC)C(=O)C=C(C)C
Mol. weight [g/mol]:	267.45

Physical Properties

Property code	Value	Unit	Source
gf	145.79	kJ/mol	Joback Method
hf	-331.83	kJ/mol	Joback Method
hfus	43.30	kJ/mol	Joback Method
hvap	62.26	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.942		Crippen Method
mcvol	257.640	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	1907.00		NIST Webbook
tb	658.71	K	Joback Method
tc	831.74	K	Joback Method
tf	344.71	K	Joback Method
vc	0.993	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.62	J/mol×K	658.71	Joback Method
cpg	739.21	J/mol×K	687.55	Joback Method
cpg	756.93	J/mol×K	716.39	Joback Method
cpg	773.80	J/mol×K	745.22	Joback Method
cpg	789.88	J/mol×K	774.06	Joback Method
cpg	805.19	J/mol×K	802.90	Joback Method
cpg	819.79	J/mol×K	831.74	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U308237&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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