

Hexanamide, N-(1-naphthyl)-

Inchi:	InChI=1S/C16H19NO/c1-2-3-4-12-16(18)17-15-11-7-9-13-8-5-6-10-14(13)15/h5-11H,2-4
InchiKey:	WWCYIHPKQXDRJX-UHFFFAOYSA-N
Formula:	C16H19NO
SMILES:	CCCCC(=O)Nc1cccc2ccccc12
Mol. weight [g/mol]:	241.33

Physical Properties

Property code	Value	Unit	Source
gf	253.74	kJ/mol	Joback Method
hf	-16.55	kJ/mol	Joback Method
hfus	34.56	kJ/mol	Joback Method
hvap	68.97	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.359		Crippen Method
mcvol	204.630	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	2226.00		NIST Webbook
tb	720.16	K	Joback Method
tc	939.93	K	Joback Method
tf	444.31	K	Joback Method
vc	0.786	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.31	J/mol×K	720.16	Joback Method
cpg	579.53	J/mol×K	756.79	Joback Method
cpg	593.74	J/mol×K	793.42	Joback Method
cpg	606.99	J/mol×K	830.05	Joback Method
cpg	619.38	J/mol×K	866.68	Joback Method
cpg	630.97	J/mol×K	903.31	Joback Method
cpg	641.85	J/mol×K	939.93	Joback Method

Sources

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=U307294&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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