Hexadecanamide

Other names:	Amide 16
	Amide HPL
	Cetyl amide
	NSC 3327
	Palmityl amide
	n-hexadecanamide
	palmitamide
	palmitic acid amide
	palmitic amide
Inchi:	InChI=1S/C16H33NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h2-15H2,1H3,(H2
InchiKey:	HSEMFIZWXHQJAE-UHFFFAOYSA-N
Formula:	C16H33NO
SMILES:	CCCCCCCCCCCCCCCC(N)=O
Mol. weight [g/mol]:	255.44
CAS:	629-54-9

Physical Properties

Property code	Value	Unit	Source
gf	21.37	kJ/mol	Joback Method
hf	-452.36	kJ/mol	Joback Method
hfus	45.40	kJ/mol	Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry
hvap	68.60	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.953		Crippen Method
mcvol	247.850	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	2142.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2182.00		NIST Webbook
rinpol	2182.00		NIST Webbook
rinpol	2144.00		NIST Webbook
rinpol	2182.00		NIST Webbook
rinpol	2186.00		NIST Webbook

rinpol	2127.00		NIST Webbook
ripol	2858.00		NIST Webbook
tb	691.88	K	Joback Method
tc	868.34	K	Joback Method
tf	380.00 ± 3.00	K	NIST Webbook
tf	380.70 ± 1.00	K	NIST Webbook
tf	311.00 ± 1.00	K	NIST Webbook
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.86	J/mol×K	691.88	Joback Method
cpg	740.44	J/mol×K	721.29	Joback Method
cpg	757.19	J/mol×K	750.70	Joback Method
cpg	773.14	J/mol×K	780.11	Joback Method
cpg	788.32	J/mol×K	809.52	Joback Method
cpg	802.75	J/mol×K	838.93	Joback Method
cpg	816.47	J/mol×K	868.34	Joback Method
hfust	45.40	kJ/mol	376.00	NIST Webbook
hsubt	181.60 ± 1.30	kJ/mol	371.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	509.20	K	1.60	NIST Webbook

Sources

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=C629549&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry:	https://www.doi.org/10.1021/je700662a

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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume