

Dodecanamide

Other names:	Amide KK Diamide Y Lauric amide Lauroylamide NSC 889 dodecamide dodecylamide lauramide lauryl amide n-Dodecanamide
Inchi:	InChI=1S/C12H25NO/c1-2-3-4-5-6-7-8-9-10-11-12(13)14/h2-11H2,1H3,(H2,13,14)
InchiKey:	ILRSCQWREDREME-UHFFFAOYSA-N
Formula:	C12H25NO
SMILES:	CCCCCCCCCCCC(N)=O
Mol. weight [g/mol]:	199.33
CAS:	1120-16-7

Physical Properties

Property code	Value	Unit	Source
gf	-12.31	kJ/mol	Joback Method
hf	-369.80	kJ/mol	Joback Method
hfus	36.30	kJ/mol	Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry
hvap	59.69	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.393		Crippen Method
mcvol	191.490	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
ripol	2784.00		NIST Webbook
ripol	2784.00		NIST Webbook
tb	600.36	K	Joback Method
tc	780.02	K	Joback Method
tf	375.00 ± 4.00	K	NIST Webbook
tf	375.30 ± 0.80	K	NIST Webbook

tf	373.15 ± 2.00	K	NIST Webbook
vc	0.743	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.17	J/mol×K	600.36	Joback Method
cpg	521.89	J/mol×K	630.30	Joback Method
cpg	536.89	J/mol×K	660.25	Joback Method
cpg	551.19	J/mol×K	690.19	Joback Method
cpg	564.82	J/mol×K	720.13	Joback Method
cpg	577.79	J/mol×K	750.08	Joback Method
cpg	590.13	J/mol×K	780.02	Joback Method
hfust	36.30	kJ/mol	373.30	NIST Webbook
hsubt	152.70 ± 0.80	kJ/mol	358.50	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=C1120167&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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