

Behenic amide

Other names:	Behenamamide Behenic acid amide Docosanamide Docsoamide Kemamide B Uniwax 1747
Inchi:	InChI=1S/C22H45NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23)2
InchiKey:	ORAWFNKFUWGRJG-UHFFFAOYSA-N
Formula:	C22H45NO
SMILES:	CCCCCCCCCCCCCCCCCCCC(=N)O
Mol. weight [g/mol]:	339.60
CAS:	3061-75-4

Physical Properties

Property code	Value	Unit	Source
gf	201.14	kJ/mol	Joback Method
hf	-451.31	kJ/mol	Joback Method
hfus	63.30	kJ/mol	Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry
hvap	93.33	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	8.344		Crippen Method
mcvol	332.390	ml/mol	McGowan Method
tb	879.28	K	Joback Method
tf	467.30	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1115.23	J/molxK	879.28	Joback Method
cpg	177.63	J/molxK	100.12	Joback Method

cpg	177.63	J/mol×K	100.12	Joback Method
cpg	177.63	J/mol×K	100.12	Joback Method
cpg	177.63	J/mol×K	100.12	Joback Method
cpg	177.63	J/mol×K	100.12	Joback Method
cpg	177.63	J/mol×K	100.12	Joback Method

Sources

Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Ethyl and Primary Alkylamides by Differential Scanning Calorimetry: McGowan Method:

<https://www.doi.org/10.1021/je700662a>

NIST Webbook:

https://en.wikipedia.org/wiki/Joback_method

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3061754&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

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
mvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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