

Hexanamide, N,N-diethyl-

Other names:	Caproic acid diethylamide N,N-Diethylhexanamide R 31
Inchi:	InChI=1S/C10H21NO/c1-4-7-8-9-10(12)11(5-2)6-3/h4-9H2,1-3H3
InchiKey:	ZZTJARSULYQEHS-UHFFFAOYSA-N
Formula:	C10H21NO
SMILES:	CCCCCC(=O)N(CC)CC
Mol. weight [g/mol]:	171.28
CAS:	6282-97-9

Physical Properties

Property code	Value	Unit	Source
gf	15.18	kJ/mol	Joback Method
hf	-294.78	kJ/mol	Joback Method
hfus	26.28	kJ/mol	Joback Method
hvap	46.64	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.435		Crippen Method
mcvol	163.310	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
tb	494.51	K	Joback Method
tc	665.67	K	Joback Method
tf	284.86	K	Joback Method
vc	0.620	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.88	J/mol×K	494.51	Joback Method
cpg	391.01	J/mol×K	523.04	Joback Method
cpg	405.50	J/mol×K	551.56	Joback Method
cpg	419.35	J/mol×K	580.09	Joback Method
cpg	432.59	J/mol×K	608.62	Joback Method
cpg	445.24	J/mol×K	637.14	Joback Method

cpg	457.30	J/mol×K	665.67	Joback Method
hvapt	47.70	kJ/mol	408.00	NIST Webbook

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=C6282979&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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