

2-propylpentanamide

Other names:	2-propylvaleramide di-n-propylacetamide
Inchi:	InChI=1S/C8H17NO/c1-3-5-7(6-4-2)8(9)10/h7H,3-6H2,1-2H3,(H2,9,10)
InchiKey:	OMOMUFTZPTXCHP-UHFFFAOYSA-N
Formula:	C8H17NO
SMILES:	CCCC(CCC)C(N)=O
Mol. weight [g/mol]:	143.23

Physical Properties

Property code	Value	Unit	Source
hf	-400.36	kJ/mol	Cheméo Relay (1.0)
hfus	19.75	kJ/mol	Joback Method
ie	9.37	eV	Cheméo Relay (1.0)
log10ws	-2.18		Cheméo Relay (1.0)
logp	1.688		Crippen Method
mcvol	135.130	ml/mol	McGowan Method
tb	473.16	K	Cheméo Relay (1.0)
tf	398.20	K	Validation of the Vaporization Enthalpies of Some Simple Aliphatic Amides and Their Use in the Evaluation of the Vaporization Enthalpy of Valpromide and Valnoctamide

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.04	J/mol×K	508.40	Joback Method
cpg	327.21	J/mol×K	540.25	Joback Method
cpg	339.77	J/mol×K	572.10	Joback Method
cpg	351.73	J/mol×K	603.95	Joback Method
cpg	363.12	J/mol×K	635.80	Joback Method
cpg	373.95	J/mol×K	667.65	Joback Method
cpg	384.23	J/mol×K	699.50	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Validation of the Vaporization Enthalpies of Some Simple Aliphatic Amides and Their Use in the Evaluation of the Vaporization Enthalpy of Valpromide and Valnoctamide: <https://www.doi.org/10.1021/je3012452>

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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