

Valnoctamide

Other names:	2-propylpentanamide 2-propylvaleramide di-n-propylacetamide
Inchi:	InChI=1S/C8H17NO/c1-4-6(3)7(5-2)8(9)10/h6-7H,4-5H2,1-3H3,(H2,9,10)
InchiKey:	QRCJOCOSPZMDJY-UHFFFAOYSA-N
Formula:	C8H17NO
SMILES:	CCC(C)C(CC)C(N)=O
Mol. weight [g/mol]:	143.23
CAS:	4171-13-5

Physical Properties

Property code	Value	Unit	Source
gf	-50.87	kJ/mol	Joback Method
hf	-297.80	kJ/mol	Joback Method
hfus	16.23	kJ/mol	Joback Method
hvap	50.01	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.544		Crippen Method
mcvol	135.130	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpola	1220.00		NIST Webbook
rinpola	1240.00		NIST Webbook
rinpola	1240.00		NIST Webbook
rinpola	1250.00		NIST Webbook
tb	507.96	K	Joback Method
tc	703.18	K	Joback Method
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
vc	0.506	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.29	J/molxK	507.96	Joback Method
cpg	327.81	J/molxK	540.50	Joback Method
cpg	340.69	J/molxK	573.03	Joback Method
cpg	352.94	J/molxK	605.57	Joback Method
cpg	364.59	J/molxK	638.11	Joback Method
cpg	375.64	J/molxK	670.65	Joback Method
cpg	386.11	J/molxK	703.18	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Validation of the Vaporization Enthalpies of Some Simple Aliphatic Amines and Their Use in the Evaluation of the Vaporization Enthalpy of Valproamide and Valnoctamide:	https://www.doi.org/10.1021/je3012452
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=C4171135&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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