

Propanamide, N-tetrahydrofurfuryl-3-chloro-

Inchi:	InChI=1S/C8H14ClNO2/c9-4-3-8(11)10-6-7-2-1-5-12-7/h7H,1-6H2,(H,10,11)
InchiKey:	OAWKSFOYJKEQCH-UHFFFAOYSA-N
Formula:	C8H14ClNO2
SMILES:	O=C(CCCI)NCC1CCCO1
Mol. weight [g/mol]:	191.66

Physical Properties

Property code	Value	Unit	Source
gf	-84.55	kJ/mol	Joback Method
hf	-354.82	kJ/mol	Joback Method
hfus	29.29	kJ/mol	Joback Method
hvap	55.74	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	0.911		Crippen Method
mcvol	142.380	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	566.14	K	Joback Method
tc	776.27	K	Joback Method
tf	349.90	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.28	J/mol×K	566.14	Joback Method
cpg	360.43	J/mol×K	601.16	Joback Method
cpg	373.73	J/mol×K	636.18	Joback Method
cpg	386.20	J/mol×K	671.20	Joback Method
cpg	397.88	J/mol×K	706.23	Joback Method
cpg	408.80	J/mol×K	741.25	Joback Method
cpg	418.99	J/mol×K	776.27	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U307224&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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