

2-Propenamide, N-(1,1-dimethylethyl)-

Other names:	Acrylamide, N-tert-butyl- N-(1,1-dimethylethyl)-2-propenamide N-(tert-butyl)acrylamide N-t-Butyl-2-propenamide N-t-Butylacrylamide N-tert-butylacrylamide tert-Butylacrylamide
Inchi:	InChI=1S/C7H13NO/c1-5-6(9)8-7(2,3)4/h5H,1H2,2-4H3,(H,8,9)
InchiKey:	XFHJDMUEHUHAJW-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	C=CC(=O)NC(C)(C)C
Mol. weight [g/mol]:	127.18
CAS:	107-58-4

Physical Properties

Property code	Value	Unit	Source
gf	59.21	kJ/mol	Joback Method
hf	-130.24	kJ/mol	Joback Method
hfus	21.57	kJ/mol	Determination and Correlation of Solubility of N-tertbutylacrylamide in Seven Different Solvents at Temperatures between (279.15 and 353.15) K
hvap	42.39	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.087		Crippen Method
mcvol	116.740	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
tb	457.05	K	Joback Method
tc	652.95	K	Joback Method
tf	271.90	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.35	J/mol×K	457.05	Joback Method
cpg	257.82	J/mol×K	489.70	Joback Method
cpg	269.55	J/mol×K	522.35	Joback Method
cpg	280.59	J/mol×K	555.00	Joback Method
cpg	290.97	J/mol×K	587.65	Joback Method
cpg	300.72	J/mol×K	620.30	Joback Method
cpg	309.87	J/mol×K	652.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination and Correlation of Solubility of N-tertbutylacrylamide in Seven Different Solvents at Temperatures between (279.15 and 353.15) K:	https://www.doi.org/10.1021/acs.jced.5b00135
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107584&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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