

Butanamide, N-isopropyl-3-methyl

Inchi:	InChI=1S/C8H17NO/c1-6(2)5-8(10)9-7(3)4/h6-7H,5H2,1-4H3,(H,9,10)
InchiKey:	WQZAOWSOYRJXOE-UHFFFAOYSA-N
Formula:	C8H17NO
SMILES:	CC(C)CC(=O)NC(C)C
Mol. weight [g/mol]:	143.23

Physical Properties

Property code	Value	Unit	Source
gf	-27.93	kJ/mol	Joback Method
hf	-278.12	kJ/mol	Joback Method
hfus	16.13	kJ/mol	Joback Method
hvap	45.81	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.557		Crippen Method
mcvol	135.130	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinsol	1088.00		NIST Webbook
tb	485.60	K	Joback Method
tc	672.00	K	Joback Method
tf	252.51	K	Joback Method
vc	0.512	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.58	J/mol×K	485.60	Joback Method
cpg	316.21	J/mol×K	516.67	Joback Method
cpg	329.23	J/mol×K	547.73	Joback Method
cpg	341.66	J/mol×K	578.80	Joback Method
cpg	353.50	J/mol×K	609.87	Joback Method
cpg	364.78	J/mol×K	640.93	Joback Method
cpg	375.50	J/mol×K	672.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R50529&Units=SI
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

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
mccvol:	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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