Butanamide, N-isobutyl-3-methyl

Inchi: InChI=1S/C9H19NO/c1-7(2)5-9(11)10-6-8(3)4/h7-8H,5-6H2,1-4H3,(H,10,11)
InchiKey: BPDCZYLPNNLOBD-UHFFFAOYSA-N
Formula: C9H19NO
SMILES: CC(C)CNC(=O)CC(C)C
Mol. weight [g/mol]: 157.25

Physical Properties

Property code	Value	Unit	Source
gf	-19.51	kJ/mol	Joback Method
hf	-298.76	kJ/mol	Joback Method
hfus	18.72	kJ/mol	Joback Method
hvap	48.03	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.805		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1218.00		NIST Webbook
tb	508.48	K	Joback Method
tc	692.88	K	Joback Method
tf	263.78	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.57	J/mol×K	508.48	Joback Method
cpg	362.09	J/mol×K	539.21	Joback Method
cpg	375.94	J/mol×K	569.95	Joback Method
cpg	389.16	J/mol×K	600.68	Joback Method
cpg	401.76	J/mol×K	631.41	Joback Method
cpg	413.76	J/mol×K	662.15	Joback Method
cpg	425.17	J/mol×K	692.88	Joback Method

Sources

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=R50501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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