Propanamide, N-butyl-2,2-dimethyl

Inchi: InChI=1S/C9H19NO/c1-5-6-7-10-8(11)9(2,3)4/h5-7H2,1-4H3,(H,10,11)
InchiKey: JSKYQRAQUAQJSW-UHFFFAOYSA-N
Formula: C9H19NO
SMILES: CCCCNC(=O)C(C)(C)C
Mol. weight [g/mol]: 157.25

Physical Properties

Property code	Value	Unit	Source
gf	-11.79	kJ/mol	Joback Method
hf	-296.95	kJ/mol	Joback Method
hfus	18.35	kJ/mol	Joback Method
hvap	47.51	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	1.949		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	1181.00		NIST Webbook
tb	506.13	K	Joback Method
tc	693.65	K	Joback Method
tf	296.20	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.11	J/mol×K	506.13	Joback Method
cpg	364.94	J/mol×K	537.38	Joback Method
cpg	379.00	J/mol×K	568.64	Joback Method
cpg	392.33	J/mol×K	599.89	Joback Method
cpg	404.94	J/mol×K	631.14	Joback Method
cpg	416.87	J/mol×K	662.40	Joback Method
cpg	428.16	J/mol×K	693.65	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=R50850&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
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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