Acetamide, N-butyl-N-3-methylbutyl-

Inchi: InChI=1S/C11H23NO/c1-5-6-8-12(11(4)13)9-7-10(2)3/h10H,5-9H2,1-4H3
InchiKey: PGJMZGOUMZZJRZ-UHFFFAOYSA-N
Formula: C11H23NO
SMILES: CCCCN(CCC(C)C)C(C)=O
Mol. weight [g/mol]: 185.31

Physical Properties

Property code	Value	Unit	Source
gf	21.16	kJ/mol	Joback Method
hf	-320.70	kJ/mol	Joback Method
hfus	25.34	kJ/mol	Joback Method
hvap	48.48	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.681		Crippen Method
mcvol	177.400	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1599.00		NIST Webbook
rinpol	1599.00		NIST Webbook
tb	516.95	K	Joback Method
tc	690.14	K	Joback Method
tf	281.13	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.60	J/mol×K	516.95	Joback Method
cpg	439.82	J/mol×K	545.82	Joback Method
cpg	455.32	J/mol×K	574.68	Joback Method
cpg	470.13	J/mol×K	603.55	Joback Method
cpg	484.26	J/mol×K	632.41	Joback Method
cpg	497.74	J/mol×K	661.28	Joback Method
cpg	510.58	J/mol×K	690.14	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=U415740&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