N-BUTYLPROPIONAMIDE

Other names: N-Butylpropanamide
Propanamide, N-butyl-
Inchi: InChI=1S/C7H15NO/c1-3-5-6-8-7(9)4-2/h3-6H2,1-2H3,(H,8,9)
InchiKey: XQZDWKBCGAJXLC-UHFFFAOYSA-N
Formula: C7H15NO
SMILES: CCCCNC(=O)CC
Mol. weight [g/mol]: 129.20

Physical Properties

Property code	Value	Unit	Source
af	0.5277		Cheméo Relay (1.0)
hf	-337.43	kJ/mol	Cheméo Relay (1.0)
hfus	20.58	kJ/mol	Joback Method
hvap	52.50	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
log10ws	-0.69		Cheméo Relay (1.0)
logp	1.313		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1185.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1185.00		NIST Webbook
tb	470.38	K	Cheméo Relay (1.0)
tc	652.99	K	Cheméo Relay (1.0)
tf	253.81	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.27	J/mol×K	463.60	Joback Method
cpg	271.21	J/mol×K	493.65	Joback Method
cpg	282.64	J/mol×K	523.71	Joback Method
cpg	293.59	J/mol×K	553.76	Joback Method

cpg	304.06	J/mol×K	583.82	Joback Method
cpg	314.06	J/mol×K	613.87	Joback Method
cpg	323.61	J/mol×K	643.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2955671&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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