Propanamide, N,N-dibutyl-2-bromo-

Inchi: InChI=1S/C11H22BrNO/c1-4-6-8-13(9-7-5-2)11(14)10(3)12/h10H,4-9H2,1-3H3
InchiKey: YODUIZXBBCYMFR-UHFFFAOYSA-N
Formula: C11H22BrNO
SMILES: CCCCN(CCCC)C(=O)C(C)Br
Mol. weight [g/mol]: 264.20

Physical Properties

Property code	Value	Unit	Source
gf	35.48	kJ/mol	Joback Method
hf	-294.37	kJ/mol	Joback Method
hfus	30.63	kJ/mol	Joback Method
hvap	54.92	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.199		Crippen Method
mcvol	194.900	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
tb	583.11	K	Joback Method
tc	769.13	K	Joback Method
tf	340.93	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.65	J/mol×K	583.11	Joback Method
cpg	487.98	J/mol×K	614.11	Joback Method
cpg	502.53	J/mol×K	645.12	Joback Method
cpg	516.33	J/mol×K	676.12	Joback Method
cpg	529.40	J/mol×K	707.12	Joback Method
cpg	541.79	J/mol×K	738.12	Joback Method
cpg	553.52	J/mol×K	769.13	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=U308371&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