Propanamide, n-decyl-N-methyl-2-bromo-

Inchi: InChI=1S/C14H28BrNO/c1-4-5-6-7-8-9-10-11-12-16(3)14(17)13(2)15/h13H,4-12H2,1-3H
InchiKey: FMDRHBOLGGPUBM-UHFFFAOYSA-N
Formula: C14H28BrNO
SMILES: CCCCCCCCCCN(C)C(=O)C(C)Br
Mol. weight [g/mol]: 306.28

Physical Properties

Property code	Value	Unit	Source
gf	60.74	kJ/mol	Joback Method
hf	-356.29	kJ/mol	Joback Method
hfus	38.40	kJ/mol	Joback Method
hvap	61.59	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.369		Crippen Method
mcvol	237.170	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	1967.00		NIST Webbook
rinpol	1967.00		NIST Webbook
tb	651.75	K	Joback Method
tc	833.02	K	Joback Method
tf	374.74	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.13	J/mol×K	651.75	Joback Method
cpg	645.90	J/mol×K	681.96	Joback Method
cpg	661.83	J/mol×K	712.17	Joback Method
cpg	676.95	J/mol×K	742.38	Joback Method
cpg	691.30	J/mol×K	772.60	Joback Method
cpg	704.92	J/mol×K	802.81	Joback Method
cpg	717.84	J/mol×K	833.02	Joback Method

Sources

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=U308374&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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