Propanamide, N,N-dinonyl-2-bromo-

Inchi: InChI=1S/C21H42BrNO/c1-4-6-8-10-12-14-16-18-23(21(24)20(3)22)19-17-15-13-11-9-7-

InchiKey: PHNYWZMKBRFRJU-UHFFFAOYSA-N

Formula: C21H42BrNO

SMILES: CCCCCCCCCN(CCCCCCCCC)C(=O)C(C)Br

Mol. weight [g/mol]: 404.47

Physical Properties

Property code	Value	Unit	Source
gf	119.68	kJ/mol	Joback Method
hf	-500.77	kJ/mol	Joback Method
hfus	56.53	kJ/mol	Joback Method
hvap	77.18	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	7.100		Crippen Method
mcvol	335.800	ml/mol	McGowan Method
pc	1043.27	kPa	Joback Method
rinpol	2550.00		NIST Webbook
rinpol	2550.00		NIST Webbook
tb	811.91	K	Joback Method
tc	997.46	K	Joback Method
tf	453.63	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.00	J/mol×K	811.91	Joback Method
cpg	1055.38	J/mol×K	842.84	Joback Method
cpg	1073.75	J/mol×K	873.76	Joback Method
cpg	1091.16	J/mol×K	904.69	Joback Method
cpg	1107.67	J/mol×K	935.61	Joback Method
cpg	1123.34	J/mol×K	966.54	Joback Method
cpg	1138.21	J/mol×K	997.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308379&Units=SI
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

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