Propanamide, N,N-diundecyl-2-bromo-

Inchi: InChI=1S/C25H50BrNO/c1-4-6-8-10-12-14-16-18-20-22-27(25(28)24(3)26)23-21-19-17-1
InchiKey: RERLSKFIOVUBMS-UHFFFAOYSA-N
Formula: C25H50BrNO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)C(C)Br
Mol. weight [g/mol]: 460.57

Physical Properties

Property code	Value	Unit	Source
gf	153.36	kJ/mol	Joback Method
hf	-583.33	kJ/mol	Joback Method
hfus	66.89	kJ/mol	Joback Method
hvap	86.08	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	8.660		Crippen Method
mcvol	392.160	ml/mol	McGowan Method
pc	825.74	kPa	Joback Method
rinpol	2979.00		NIST Webbook
tb	903.43	K	Joback Method
tc	1106.73	K	Joback Method
tf	498.71	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.63	J/mol×K	903.43	Joback Method
cpg	1309.12	J/mol×K	937.31	Joback Method
cpg	1329.41	J/mol×K	971.20	Joback Method
cpg	1348.56	J/mol×K	1005.08	Joback Method
cpg	1366.68	J/mol×K	1038.96	Joback Method
cpg	1383.83	J/mol×K	1072.85	Joback Method
cpg	1400.10	J/mol×K	1106.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308381&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