Propanamide, N,N-didecyl-2-bromo-

Inchi: InChI=1S/C23H46BrNO/c1-4-6-8-10-12-14-16-18-20-25(23(26)22(3)24)21-19-17-15-13-1
InchiKey: RJTSNDBRYKRGKA-UHFFFAOYSA-N
Formula: C23H46BrNO
SMILES: CCCCCCCCCCN(CCCCCCCCCC)C(=O)C(C)Br
Mol. weight [g/mol]: 432.52

Physical Properties

Property code	Value	Unit	Source
gf	136.52	kJ/mol	Joback Method
hf	-542.05	kJ/mol	Joback Method
hfus	61.71	kJ/mol	Joback Method
hvap	81.63	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	7.880		Crippen Method
mcvol	363.980	ml/mol	McGowan Method
pc	924.99	kPa	Joback Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
tb	857.67	K	Joback Method
tc	1050.33	K	Joback Method
tf	476.17	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1160.43	J/mol×K	857.67	Joback Method
cpg	1180.75	J/mol×K	889.78	Joback Method
cpg	1199.98	J/mol×K	921.89	Joback Method
cpg	1218.17	J/mol×K	954.00	Joback Method
cpg	1235.41	J/mol×K	986.11	Joback Method
cpg	1251.74	J/mol×K	1018.22	Joback Method
cpg	1267.24	J/mol×K	1050.33	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=U308380&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