Hexanamide, N,N-didecyl-6-bromo-

Inchi: InChI=1S/C26H52BrNO/c1-3-5-7-9-11-13-15-20-24-28(26(29)22-18-17-19-23-27)25-21-1
InchiKey: ABYHXIDXYXTZBH-UHFFFAOYSA-N
Formula: C26H52BrNO
SMILES: CCCCCCCCCCN(CCCCCCCCCC)C(=O)CCCCCBr
Mol. weight [g/mol]: 474.60

Physical Properties

Property code	Value	Unit	Source
gf	164.22	kJ/mol	Joback Method
hf	-598.69	kJ/mol	Joback Method
hfus	73.00	kJ/mol	Joback Method
hvap	88.69	kJ/mol	Joback Method
log10ws	-9.48		Crippen Method
logp	9.052		Crippen Method
mcvol	406.250	ml/mol	McGowan Method
pc	778.51	kPa	Joback Method
rinpol	3175.00		NIST Webbook
tb	926.75	K	Joback Method
tc	1137.89	K	Joback Method
tf	524.98	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1351.78	J/mol×K	926.75	Joback Method
cpg	1374.10	J/mol×K	961.94	Joback Method
cpg	1395.15	J/mol×K	997.13	Joback Method
cpg	1415.02	J/mol×K	1032.32	Joback Method
cpg	1433.79	J/mol×K	1067.51	Joback Method
cpg	1451.58	J/mol×K	1102.70	Joback Method
cpg	1468.47	J/mol×K	1137.89	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=U308654&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