Hexanamide, N,N-dihexyl-6-bromo-

Inchi: InChI=1S/C18H36BrNO/c1-3-5-7-12-16-20(17-13-8-6-4-2)18(21)14-10-9-11-15-19/h3-17
InchiKey: SXKOXSZLUVBISJ-UHFFFAOYSA-N
Formula: C18H36BrNO
SMILES: CCCCCCN(CCCCCC)C(=O)CCCCCBr
Mol. weight [g/mol]: 362.39

Physical Properties

Property code	Value	Unit	Source
gf	96.86	kJ/mol	Joback Method
hf	-433.57	kJ/mol	Joback Method
hfus	52.28	kJ/mol	Joback Method
hvap	70.89	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.931		Crippen Method
mcvol	293.530	ml/mol	McGowan Method
pc	1261.06	kPa	Joback Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	743.71	K	Joback Method
tc	922.40	K	Joback Method
tf	434.82	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.05	J/mol×K	743.71	Joback Method
cpg	873.10	J/mol×K	773.49	Joback Method
cpg	890.25	J/mol×K	803.27	Joback Method
cpg	906.54	J/mol×K	833.05	Joback Method
cpg	922.03	J/mol×K	862.83	Joback Method
cpg	936.75	J/mol×K	892.62	Joback Method
cpg	950.74	J/mol×K	922.40	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=U308649&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