Hexanamide, N,N-diundecyl-6-bromo-

Inchi: InChI=1S/C28H56BrNO/c1-3-5-7-9-11-13-15-17-22-26-30(28(31)24-20-19-21-25-29)27-2
InchiKey: YTUVWMGIUYOONX-UHFFFAOYSA-N
Formula: C28H56BrNO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)CCCCCBr
Mol. weight [g/mol]: 502.65

Physical Properties

Property code	Value	Unit	Source
gf	181.06	kJ/mol	Joback Method
hf	-639.97	kJ/mol	Joback Method
hfus	78.18	kJ/mol	Joback Method
hvap	93.15	kJ/mol	Joback Method
log10ws	-10.32		Crippen Method
logp	9.832		Crippen Method
mcvol	434.430	ml/mol	McGowan Method
pc	701.35	kPa	Joback Method
rinpol	3577.00		NIST Webbook
rinpol	3577.00		NIST Webbook
tb	972.51	K	Joback Method
tc	1201.61	K	Joback Method
tf	547.52	K	Joback Method
vc	1.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1482.50	J/mol×K	972.51	Joback Method
cpg	1506.59	J/mol×K	1010.69	Joback Method
cpg	1529.22	J/mol×K	1048.88	Joback Method
cpg	1550.52	J/mol×K	1087.06	Joback Method
cpg	1570.62	J/mol×K	1125.24	Joback Method
cpg	1589.65	J/mol×K	1163.42	Joback Method
cpg	1607.75	J/mol×K	1201.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308655&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

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