Pentanamide, N,N-dibutyl-5-bromo-

Inchi: InChI=1S/C13H26BrNO/c1-3-5-11-15(12-6-4-2)13(16)9-7-8-10-14/h3-12H2,1-2H3
InchiKey: YZXXOVLXZCQHGQ-UHFFFAOYSA-N
Formula: C13H26BrNO
SMILES: CCCCN(CCCC)C(=O)CCCCBr
Mol. weight [g/mol]: 292.26

Physical Properties

Property code	Value	Unit	Source
gf	54.76	kJ/mol	Joback Method
hf	-330.37	kJ/mol	Joback Method
hfus	39.33	kJ/mol	Joback Method
hvap	59.76	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.980		Crippen Method
mcvol	223.080	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1883.00		NIST Webbook
tb	629.31	K	Joback Method
tc	808.93	K	Joback Method
tf	378.47	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.15	J/mol×K	629.31	Joback Method
cpg	591.20	J/mol×K	659.25	Joback Method
cpg	606.45	J/mol×K	689.18	Joback Method
cpg	620.94	J/mol×K	719.12	Joback Method
cpg	634.71	J/mol×K	749.05	Joback Method
cpg	647.78	J/mol×K	778.99	Joback Method
cpg	660.20	J/mol×K	808.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308258&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