Pentanamide, N,N-didecyl-5-bromo-

Inchi: InChI=1S/C25H50BrNO/c1-3-5-7-9-11-13-15-19-23-27(25(28)21-17-18-22-26)24-20-16-1
InchiKey: ONNQWNPQXXXNQD-UHFFFAOYSA-N
Formula: C25H50BrNO
SMILES: CCCCCCCCCCN(CCCCCCCCCC)C(=O)CCCCBr
Mol. weight [g/mol]: 460.57

Physical Properties

Property code	Value	Unit	Source
gf	155.80	kJ/mol	Joback Method
hf	-578.05	kJ/mol	Joback Method
hfus	70.41	kJ/mol	Joback Method
hvap	86.47	kJ/mol	Joback Method
log10ws	-9.06		Crippen Method
logp	8.662		Crippen Method
mcvol	392.160	ml/mol	McGowan Method
pc	821.95	kPa	Joback Method
rinpol	3127.00		NIST Webbook
rinpol	3127.00		NIST Webbook
tb	903.87	K	Joback Method
tc	1107.79	K	Joback Method
tf	513.71	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.24	J/mol×K	903.87	Joback Method
cpg	1308.81	J/mol×K	937.86	Joback Method
cpg	1329.19	J/mol×K	971.84	Joback Method
cpg	1348.45	J/mol×K	1005.83	Joback Method
cpg	1366.67	J/mol×K	1039.81	Joback Method
cpg	1383.93	J/mol×K	1073.80	Joback Method
cpg	1400.32	J/mol×K	1107.79	Joback Method

Sources

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=U308267&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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