Pentanamide, N,N-dinonyl-5-bromo-

Inchi: InChI=1S/C23H46BrNO/c1-3-5-7-9-11-13-17-21-25(23(26)19-15-16-20-24)22-18-14-12-1
InchiKey: NXBDCOMWLLINIX-UHFFFAOYSA-N
Formula: C23H46BrNO
SMILES: CCCCCCCCCN(CCCCCCCCC)C(=O)CCCCBr
Mol. weight [g/mol]: 432.52

Physical Properties

Property code	Value	Unit	Source
gf	138.96	kJ/mol	Joback Method
hf	-536.77	kJ/mol	Joback Method
hfus	65.23	kJ/mol	Joback Method
hvap	82.02	kJ/mol	Joback Method
log10ws	-8.23		Crippen Method
logp	7.881		Crippen Method
mcvol	363.980	ml/mol	McGowan Method
pc	920.50	kPa	Joback Method
rinpol	2868.00		NIST Webbook
rinpol	2868.00		NIST Webbook
tb	858.11	K	Joback Method
tc	1050.65	K	Joback Method
tf	491.17	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1159.99	J/mol×K	858.11	Joback Method
cpg	1180.31	J/mol×K	890.20	Joback Method
cpg	1199.54	J/mol×K	922.29	Joback Method
cpg	1217.76	J/mol×K	954.38	Joback Method
cpg	1235.03	J/mol×K	986.47	Joback Method
cpg	1251.41	J/mol×K	1018.56	Joback Method
cpg	1266.97	J/mol×K	1050.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308266&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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