Benzamide, N,N-dioctyl-3-bromo-

Inchi: InChI=1S/C23H38BrNO/c1-3-5-7-9-11-13-18-25(19-14-12-10-8-6-4-2)23(26)21-16-15-17
InchiKey: LBOYEDQYTMLKPI-UHFFFAOYSA-N
Formula: C23H38BrNO
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 424.46

Physical Properties

Property code	Value	Unit	Source
gf	241.74	kJ/mol	Joback Method
hf	-311.71	kJ/mol	Joback Method
hfus	58.88	kJ/mol	Joback Method
hvap	84.95	kJ/mol	Joback Method
log10ws	-8.64		Crippen Method
logp	7.612		Crippen Method
mcvol	340.220	ml/mol	McGowan Method
pc	1126.08	kPa	Joback Method
rinpol	2731.00		NIST Webbook
rinpol	2731.00		NIST Webbook
tb	889.77	K	Joback Method
tc	1094.17	K	Joback Method
tf	530.11	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.09	J/mol×K	889.77	Joback Method
cpg	1084.04	J/mol×K	923.84	Joback Method
cpg	1100.94	J/mol×K	957.90	Joback Method
cpg	1116.86	J/mol×K	991.97	Joback Method
cpg	1131.87	J/mol×K	1026.03	Joback Method
cpg	1146.07	J/mol×K	1060.10	Joback Method
cpg	1159.51	J/mol×K	1094.17	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=U308627&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