Benzamide, N,N-diheptyl-4-bromo-

Inchi: InChI=1S/C21H34BrNO/c1-3-5-7-9-11-17-23(18-12-10-8-6-4-2)21(24)19-13-15-20(22)16
InchiKey: KDHOBSZTEKBRDU-UHFFFAOYSA-N
Formula: C21H34BrNO
SMILES: CCCCCCCN(CCCCCCC)C(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 396.40

Physical Properties

Property code	Value	Unit	Source
gf	224.90	kJ/mol	Joback Method
hf	-270.43	kJ/mol	Joback Method
hfus	53.70	kJ/mol	Joback Method
hvap	80.50	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	6.832		Crippen Method
mcvol	312.040	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	2632.00		NIST Webbook
tb	844.01	K	Joback Method
tc	1045.57	K	Joback Method
tf	507.57	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.83	J/mol×K	844.01	Joback Method
cpg	962.19	J/mol×K	877.60	Joback Method
cpg	978.53	J/mol×K	911.20	Joback Method
cpg	993.91	J/mol×K	944.79	Joback Method
cpg	1008.40	J/mol×K	978.39	Joback Method
cpg	1022.08	J/mol×K	1011.98	Joback Method
cpg	1035.01	J/mol×K	1045.57	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308456&Units=SI

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