Benzamide, N-heptyl-N-octyl-3-bromo-

Inchi: InChI=1S/C22H36BrNO/c1-3-5-7-9-11-13-18-24(17-12-10-8-6-4-2)22(25)20-15-14-16-21
InchiKey: RPMOQVIHJDQPPK-UHFFFAOYSA-N
Formula: C22H36BrNO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 410.43

Physical Properties

Property code	Value	Unit	Source
gf	233.32	kJ/mol	Joback Method
hf	-291.07	kJ/mol	Joback Method
hfus	56.29	kJ/mol	Joback Method
hvap	82.73	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	7.222		Crippen Method
mcvol	326.130	ml/mol	McGowan Method
pc	1202.29	kPa	Joback Method
rinpol	2629.00		NIST Webbook
tb	866.89	K	Joback Method
tc	1069.49	K	Joback Method
tf	518.84	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.09	J/mol×K	866.89	Joback Method
cpg	1022.73	J/mol×K	900.66	Joback Method
cpg	1039.33	J/mol×K	934.42	Joback Method
cpg	1054.97	J/mol×K	968.19	Joback Method
cpg	1069.71	J/mol×K	1001.96	Joback Method
cpg	1083.64	J/mol×K	1035.72	Joback Method
cpg	1096.82	J/mol×K	1069.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308626&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