Benzamide, N,N-bis(2-ethylhexyl)-4-bromo-

Inchi: InChI=1S/C23H38BrNO/c1-5-9-11-19(7-3)17-25(18-20(8-4)12-10-6-2)23(26)21-13-15-22
InchiKey: UULVFHPSDGTSMF-UHFFFAOYSA-N
Formula: C23H38BrNO
SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 424.46

Physical Properties

Property code	Value	Unit	Source
gf	236.86	kJ/mol	Joback Method
hf	-322.27	kJ/mol	Joback Method
hfus	51.84	kJ/mol	Joback Method
hvap	84.18	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	7.324		Crippen Method
mcvol	340.220	ml/mol	McGowan Method
pc	1138.27	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
tb	888.89	K	Joback Method
tc	1095.74	K	Joback Method
tf	500.11	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.01	J/mol×K	888.89	Joback Method
cpg	1085.12	J/mol×K	923.36	Joback Method
cpg	1102.13	J/mol×K	957.84	Joback Method
cpg	1118.12	J/mol×K	992.31	Joback Method
cpg	1133.16	J/mol×K	1026.79	Joback Method
cpg	1147.33	J/mol×K	1061.26	Joback Method
cpg	1160.73	J/mol×K	1095.74	Joback Method

Sources

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=U308455&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

https://www.chemeo.com/cid/99-189-4/Benzamide-N-N-bis-2-ethylhexyl-4-bromo.pdf

Generated by Cheméo on 2024-10-12 02:16:03.416356934 +0000 UTC m=+3280226.053326182.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.