

Benzamide, 2-bromo-N-ethyl-N-dodecyl-

Inchi:	InChI=1S/C21H34BrNO/c1-3-5-6-7-8-9-10-11-12-15-18-23(4-2)21(24)19-16-13-14-17-20
InchiKey:	CXOPPVRTXKIOIO-UHFFFAOYSA-N
Formula:	C21H34BrNO
SMILES:	CCCCCCCCCCCCN(CC)C(=O)c1ccccc1Br
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
mvol	312.040	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	3162.00		NIST Webbook
rinpol	3162.00		NIST Webbook
tb	844.01	K	Joback Method
tc	1045.57	K	Joback Method
tf	507.57	K	Joback Method
vc	1.190	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U415367&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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