

Benzamide, N,N-didecyl-4-bromo-

Inchi: InChI=1S/C27H46BrNO/c1-3-5-7-9-11-13-15-17-23-29(24-18-16-14-12-10-8-6-4-2)27(30)
InchiKey: FCCLJZZSCUIGPH-UHFFFAOYSA-N
Formula: C27H46BrNO
SMILES: CCCCCCCCCCN(CCCCCCCCCC)C(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 480.56

Physical Properties

Property code	Value	Unit	Source
gf	275.42	kJ/mol	Joback Method
hf	-394.27	kJ/mol	Joback Method
hfus	69.24	kJ/mol	Joback Method
hvap	93.86	kJ/mol	Joback Method
log10ws	-10.31		Crippen Method
logp	9.173		Crippen Method
mcvol	396.580	ml/mol	McGowan Method
pc	883.67	kPa	Joback Method
rinpol	3479.00		NIST Webbook
rinpol	3479.00		NIST Webbook
tb	981.29	K	Joback Method
tc	1201.73	K	Joback Method
tf	575.19	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1316.66	J/mol×K	981.29	Joback Method
cpg	1336.34	J/mol×K	1018.03	Joback Method
cpg	1354.84	J/mol×K	1054.77	Joback Method
cpg	1372.28	J/mol×K	1091.51	Joback Method
cpg	1388.77	J/mol×K	1128.25	Joback Method
cpg	1404.41	J/mol×K	1164.99	Joback Method
cpg	1419.33	J/mol×K	1201.73	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=U308460&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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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