Benzamide, N,N-diundecyl-3-bromo-

Inchi: InChI=1S/C29H50BrNO/c1-3-5-7-9-11-13-15-17-19-24-31(29(32)27-22-21-23-28(30)26-2
InchiKey: JXRJQTVTCGKAIP-UHFFFAOYSA-N
Formula: C29H50BrNO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 508.62

Physical Properties

Property code	Value	Unit	Source
gf	292.26	kJ/mol	Joback Method
hf	-435.55	kJ/mol	Joback Method
hfus	74.42	kJ/mol	Joback Method
hvap	98.31	kJ/mol	Joback Method
log10ws	-11.15		Crippen Method
logp	9.953		Crippen Method
mcvol	424.760	ml/mol	McGowan Method
pc	790.82	kPa	Joback Method
rinpol	3693.00		NIST Webbook
rinpol	3693.00		NIST Webbook
tb	1027.05	K	Joback Method
tc	1261.79	K	Joback Method
tf	597.73	K	Joback Method
vc	1.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1445.33	J/mol×K	1027.05	Joback Method
cpg	1466.29	J/mol×K	1066.17	Joback Method
cpg	1485.98	J/mol×K	1105.30	Joback Method
cpg	1504.55	J/mol×K	1144.42	Joback Method
cpg	1522.14	J/mol×K	1183.54	Joback Method
cpg	1538.89	J/mol×K	1222.66	Joback Method
cpg	1554.95	J/mol×K	1261.79	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=U308630&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