

Benzamide, 4-butyl-N-butyl-N-tetradecyl-

Inchi: InChI=1S/C29H51NO/c1-4-7-10-11-12-13-14-15-16-17-18-19-26-30(25-9-6-3)29(31)28-2
InchiKey: XRWIPWXAGZMEOH-UHFFFAOYSA-N
Formula: C29H51NO
SMILES: CCCCCCCCCCCCCCN(CCCC)C(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 429.72

Physical Properties

Property code	Value	Unit	Source
gf	277.94	kJ/mol	Joback Method
hf	-461.88	kJ/mol	Joback Method
hfus	69.14	kJ/mol	Joback Method
hvap	91.87	kJ/mol	Joback Method
log10ws	-9.95		Crippen Method
logp	8.973		Crippen Method
mcvol	407.260	ml/mol	McGowan Method
pc	761.00	kPa	Joback Method
rinpol	2058.00		NIST Webbook
rinpol	2058.00		NIST Webbook
tb	960.89	K	Joback Method
tc	1178.19	K	Joback Method
tf	537.93	K	Joback Method
vc	1.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1397.40	J/mol×K	960.89	Joback Method
cpg	1419.26	J/mol×K	997.11	Joback Method
cpg	1439.75	J/mol×K	1033.32	Joback Method
cpg	1458.96	J/mol×K	1069.54	Joback Method
cpg	1476.99	J/mol×K	1105.75	Joback Method
cpg	1493.96	J/mol×K	1141.97	Joback Method
cpg	1509.95	J/mol×K	1178.19	Joback Method

Sources

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=U415884&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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