

Benzamide, 4-chloro-N-ethyl-N-hexadecyl-

Inchi:

InChI=1S/C25H42ClNO/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-22-27(4-2)25(28)23-18

InchiKey:

WTPOCVBIHOAMHI-UHFFFAOYSA-N

Formula:

C25H42ClNO

SMILES:

CCCCCCCCCCCCCCCCCN(CC)C(=O)c1ccc(Cl)cc1

Mol. weight [g/mol]:

408.06

Physical Properties

Property code	Value	Unit	Source
gf	232.33	kJ/mol	Joback Method
hf	-395.06	kJ/mol	Joback Method
hfus	62.98	kJ/mol	Joback Method
hvap	87.36	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	8.283		Crippen Method
mcvol	363.140	ml/mol	McGowan Method
pc	930.64	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1533.00		NIST Webbook
tb	906.80	K	Joback Method
tc	1111.03	K	Joback Method
tf	522.77	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1173.40	J/mol×K	906.80	Joback Method
cpg	1192.45	J/mol×K	940.84	Joback Method
cpg	1210.35	J/mol×K	974.88	Joback Method
cpg	1227.16	J/mol×K	1008.92	Joback Method
cpg	1242.97	J/mol×K	1042.96	Joback Method
cpg	1257.85	J/mol×K	1077.00	Joback Method
cpg	1271.88	J/mol×K	1111.03	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=U415336&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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