

Benzamide, N,N-diundecyl-4-chloro-

Inchi:	InChI=1S/C29H50ClNO/c1-3-5-7-9-11-13-15-17-19-25-31(29(32)27-21-23-28(30)24-22-2
InchiKey:	IXVPONKEZNEHKB-UHFFFAOYSA-N
Formula:	C29H50ClNO
SMILES:	CCCCCCCCCCCCN(CCCCCCCCCCCC)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	464.17

Physical Properties

Property code	Value	Unit	Source
gf	266.01	kJ/mol	Joback Method
hf	-477.62	kJ/mol	Joback Method
hfus	73.33	kJ/mol	Joback Method
hvap	96.26	kJ/mol	Joback Method
log10ws	-10.67		Crippen Method
logp	9.844		Crippen Method
mcvol	419.500	ml/mol	McGowan Method
pc	745.70	kPa	Joback Method
rinpol	3546.00		NIST Webbook
tb	998.32	K	Joback Method
tc	1226.05	K	Joback Method
tf	567.85	K	Joback Method
vc	1.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1428.25	J/mol×K	998.32	Joback Method
cpg	1449.39	J/mol×K	1036.28	Joback Method
cpg	1469.15	J/mol×K	1074.23	Joback Method
cpg	1487.66	J/mol×K	1112.19	Joback Method
cpg	1505.04	J/mol×K	1150.14	Joback Method
cpg	1521.42	J/mol×K	1188.10	Joback Method
cpg	1536.91	J/mol×K	1226.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308595&Units=SI
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

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

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