

Phenylacetamide, N,N-diundecyl-

Inchi:	InChI=1S/C30H53NO/c1-3-5-7-9-11-13-15-17-22-26-31(30(32)28-29-24-20-19-21-25-29)
InchiKey:	UFECKRKOXAPZFG-UHFFFAOYSA-N
Formula:	C30H53NO
SMILES:	CCCCCCCCCCCN(CCCCCCCCCC)C(=O)Cc1ccccc1
Mol. weight [g/mol]:	443.75

Physical Properties

Property code	Value	Unit	Source
gf	295.99	kJ/mol	Joback Method
hf	-471.05	kJ/mol	Joback Method
hfus	72.12	kJ/mol	Joback Method
hvap	93.44	kJ/mol	Joback Method
log10ws	-9.83		Crippen Method
logp	9.119		Crippen Method
mcvol	421.350	ml/mol	McGowan Method
pc	728.10	kPa	Joback Method
rinsol	3554.00		NIST Webbook
tb	978.79	K	Joback Method
tc	1202.42	K	Joback Method
tf	536.68	K	Joback Method
vc	1.631	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.54	J/mol×K	978.79	Joback Method
cpg	1485.13	J/mol×K	1016.06	Joback Method
cpg	1506.29	J/mol×K	1053.33	Joback Method
cpg	1526.15	J/mol×K	1090.60	Joback Method
cpg	1544.82	J/mol×K	1127.88	Joback Method
cpg	1562.43	J/mol×K	1165.15	Joback Method
cpg	1579.11	J/mol×K	1202.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308416&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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