Phenylacetamide, N,N-didecyl-

Inchi: InChI=1S/C28H49NO/c1-3-5-7-9-11-13-15-20-24-29(25-21-16-14-12-10-8-6-4-2)28(30)2
InchiKey: RDFQZGXJPRGHMM-UHFFFAOYSA-N
Formula: C28H49NO
SMILES: CCCCCCCCCCN(CCCCCCCCCC)C(=O)Cc1ccccc1
Mol. weight [g/mol]: 415.69

Physical Properties

Property code	Value	Unit	Source
gf	279.15	kJ/mol	Joback Method
hf	-429.77	kJ/mol	Joback Method
hfus	66.94	kJ/mol	Joback Method
hvap	88.99	kJ/mol	Joback Method
log10ws	-8.99		Crippen Method
logp	8.339		Crippen Method
mcvol	393.170	ml/mol	McGowan Method
pc	809.83	kPa	Joback Method
rinpol	3157.00		NIST Webbook
tb	933.03	K	Joback Method
tc	1142.61	K	Joback Method
tf	514.14	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.59	J/mol×K	933.03	Joback Method
cpg	1353.95	J/mol×K	967.96	Joback Method
cpg	1374.01	J/mol×K	1002.89	Joback Method
cpg	1392.86	J/mol×K	1037.82	Joback Method
cpg	1410.61	J/mol×K	1072.75	Joback Method
cpg	1427.34	J/mol×K	1107.68	Joback Method
cpg	1443.16	J/mol×K	1142.61	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=U308415&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
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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