Pentanamide, N,N-diundecyl-

Inchi: InChI=1S/C27H55NO/c1-4-7-10-12-14-16-18-20-22-25-28(27(29)24-9-6-3)26-23-21-19-1
InchiKey: HBEHPZKSJAMBPI-UHFFFAOYSA-N
Formula: C27H55NO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)CCCC
Mol. weight [g/mol]: 409.73

Physical Properties

Property code	Value	Unit	Source
gf	158.32	kJ/mol	Joback Method
hf	-645.66	kJ/mol	Joback Method
hfus	70.31	kJ/mol	Joback Method
hvap	84.48	kJ/mol	Joback Method
log10ws	-9.47		Crippen Method
logp	9.067		Crippen Method
mcvol	402.840	ml/mol	McGowan Method
pc	711.49	kPa	Joback Method
rinpol	2920.00		NIST Webbook
rinpol	2920.00		NIST Webbook
tb	883.47	K	Joback Method
tc	1084.86	K	Joback Method
tf	476.45	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1361.50	J/mol×K	883.47	Joback Method
cpg	1385.56	J/mol×K	917.03	Joback Method
cpg	1408.26	J/mol×K	950.60	Joback Method
cpg	1429.66	J/mol×K	984.16	Joback Method
cpg	1449.85	J/mol×K	1017.73	Joback Method
cpg	1468.90	J/mol×K	1051.29	Joback Method
cpg	1486.88	J/mol×K	1084.86	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=U308188&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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