Octanamide, N,N-diundecyl-

Inchi: InChI=1S/C30H61NO/c1-4-7-10-13-15-17-19-22-25-28-31(30(32)27-24-21-12-9-6-3)29-2
InchiKey: RWTTZNZXOQZQRN-UHFFFAOYSA-N
Formula: C30H61NO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)CCCCCCC
Mol. weight [g/mol]: 451.81

Physical Properties

Property code	Value	Unit	Source
gf	183.58	kJ/mol	Joback Method
hf	-707.58	kJ/mol	Joback Method
hfus	78.08	kJ/mol	Joback Method
hvap	91.16	kJ/mol	Joback Method
log10ws	-10.73		Crippen Method
logp	10.237		Crippen Method
mcvol	445.110	ml/mol	McGowan Method
pc	613.60	kPa	Joback Method
rinpol	3334.00		NIST Webbook
rinpol	3334.00		NIST Webbook
tb	952.11	K	Joback Method
tc	1181.94	K	Joback Method
tf	510.26	K	Joback Method
vc	1.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1560.74	J/mol×K	952.11	Joback Method
cpg	1587.65	J/mol×K	990.41	Joback Method
cpg	1612.82	J/mol×K	1028.72	Joback Method
cpg	1636.39	J/mol×K	1067.02	Joback Method
cpg	1658.48	J/mol×K	1105.33	Joback Method
cpg	1679.21	J/mol×K	1143.63	Joback Method
cpg	1698.72	J/mol×K	1181.94	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=U308449&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