Octanamide, N,N-diheptyl-

Inchi: InChI=1S/C22H45NO/c1-4-7-10-13-16-19-22(24)23(20-17-14-11-8-5-2)21-18-15-12-9-6-3

InchiKey: YNQDXMVJQLCEHI-UHFFFAOYSA-N

Formula: C22H45NO

SMILES: CCCCCCCC(=O)N(CCCCCCC)CCCCCCC

Mol. weight [g/mol]: 339.60

Physical Properties

Property code	Value	Unit	Source
gf	116.22	kJ/mol	Joback Method
hf	-542.46	kJ/mol	Joback Method
hfus	57.36	kJ/mol	Joback Method
hvap	73.36	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	7.116		Crippen Method
mcvol	332.390	ml/mol	McGowan Method
pc	935.77	kPa	Joback Method
rinpol	2401.00		NIST Webbook
rinpol	2401.00		NIST Webbook
tb	769.07	K	Joback Method
tc	943.91	K	Joback Method
tf	420.10	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.20	J/mol×K	769.07	Joback Method
cpg	1062.13	J/mol×K	798.21	Joback Method
cpg	1082.04	J/mol×K	827.35	Joback Method
cpg	1100.97	J/mol×K	856.49	Joback Method
cpg	1118.97	J/mol×K	885.63	Joback Method
cpg	1136.08	J/mol×K	914.77	Joback Method
cpg	1152.33	J/mol×K	943.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308444&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

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