Octanamide, N,N-dinonyl-

Inchi: InChI=1S/C26H53NO/c1-4-7-10-13-15-18-21-24-27(25-22-19-16-14-11-8-5-2)26(28)23-2
InchiKey: BTQILVQTQBZOGO-UHFFFAOYSA-N
Formula: C26H53NO
SMILES: CCCCCCCCCN(CCCCCCCCC)C(=O)CCCCCCC
Mol. weight [g/mol]: 395.71

Physical Properties

Property code	Value	Unit	Source
gf	149.90	kJ/mol	Joback Method
hf	-625.02	kJ/mol	Joback Method
hfus	67.72	kJ/mol	Joback Method
hvap	82.26	kJ/mol	Joback Method
log10ws	-9.05		Crippen Method
logp	8.677		Crippen Method
mcvol	388.750	ml/mol	McGowan Method
pc	749.38	kPa	Joback Method
rinpol	2789.00		NIST Webbook
rinpol	2789.00		NIST Webbook
tb	860.59	K	Joback Method
tc	1054.80	K	Joback Method
tf	465.18	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1296.13	J/mol×K	860.59	Joback Method
cpg	1319.43	J/mol×K	892.96	Joback Method
cpg	1341.45	J/mol×K	925.33	Joback Method
cpg	1362.26	J/mol×K	957.70	Joback Method
cpg	1381.93	J/mol×K	990.07	Joback Method
cpg	1400.51	J/mol×K	1022.44	Joback Method
cpg	1418.09	J/mol×K	1054.80	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=U308447&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