N-Stearoyldextramine

Inchi: InChI=1S/C27H46N2O5/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-26(31)28-25(22-30
InchiKey: ULVKSVBYCYGJMG-UHFFFAOYSA-N
Formula: C27H46N2O5
SMILES: CCCCCCCCCCCCCCCCCC(=O)NC(CO)C(O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 478.66
CAS: 36136-05-7

Physical Properties

Property code	Value	Unit	Source
chs	-16133.71	kJ/mol	NIST Webbook
gf	-3.26	kJ/mol	Joback Method
hf	-760.44	kJ/mol	Joback Method
hfus	78.53	kJ/mol	Joback Method
hvap	140.99	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	6.367		Crippen Method
mcvol	408.240	ml/mol	McGowan Method
pc	972.91	kPa	Joback Method
tb	1288.18	K	Joback Method
tc	1663.96	K	Joback Method
tf	770.83	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.06	J/mol×K	1288.18	Joback Method
cpg	1540.31	J/mol×K	1350.81	Joback Method
cpg	1558.26	J/mol×K	1413.44	Joback Method
cpg	1575.45	J/mol×K	1476.07	Joback Method
cpg	1592.38	J/mol×K	1538.70	Joback Method
cpg	1609.58	J/mol×K	1601.33	Joback Method
cpg	1627.56	J/mol×K	1663.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36136057&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume