Carbonic acid, monoamide, N-octadecyl-, octyl ester

Inchi: InChI=1S/C27H55NO2/c1-3-5-7-9-11-12-13-14-15-16-17-18-19-20-21-23-25-28-27(29)30
InchiKey: OEEWTACEHHRHGE-UHFFFAOYSA-N
Formula: C27H55NO2
SMILES: CCCCCCCCCCCCCCCCCCCNC(=O)OCCCCCCCC
Mol. weight [g/mol]: 425.73

Physical Properties

Property code	Value	Unit	Source
gf	31.93	kJ/mol	Joback Method
hf	-791.94	kJ/mol	Joback Method
hfus	73.57	kJ/mol	Joback Method
hvap	91.29	kJ/mol	Joback Method
log10ws	-10.15		Crippen Method
logp	9.335		Crippen Method
mcvol	408.710	ml/mol	McGowan Method
pc	710.73	kPa	Joback Method
rinpol	3132.00		NIST Webbook
rinpol	3132.00		NIST Webbook
tb	943.62	K	Joback Method
tc	1165.23	K	Joback Method
tf	518.87	K	Joback Method
vc	1.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1421.14	J/mol×K	943.62	Joback Method
cpg	1444.87	J/mol×K	980.55	Joback Method
cpg	1466.94	J/mol×K	1017.49	Joback Method
cpg	1487.43	J/mol×K	1054.42	Joback Method
cpg	1506.41	J/mol×K	1091.36	Joback Method
cpg	1523.97	J/mol×K	1128.29	Joback Method
cpg	1540.17	J/mol×K	1165.23	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=U406839&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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