Carbonic acid, monoamide, N-dodecyl-, propyl ester

Inchi: InChI=1S/C16H33NO2/c1-3-5-6-7-8-9-10-11-12-13-14-17-16(18)19-15-4-2/h3-15H2,1-2H

InchiKey: VPZKJMRKDZHNPR-UHFFFAOYSA-N

Formula: C16H33NO2

SMILES: CCCCCCCCCCCCNC(=O)OCCC

Mol. weight [g/mol]: 271.44

Physical Properties

Property code	Value	Unit	Source
gf	-60.69	kJ/mol	Joback Method
hf	-564.90	kJ/mol	Joback Method
hfus	45.08	kJ/mol	Joback Method
hvap	66.80	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.043		Crippen Method
mcvol	253.720	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook
tb	691.94	K	Joback Method
tc	863.46	K	Joback Method
tf	394.90	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.21	J/mol×K	691.94	Joback Method
cpg	756.82	J/mol×K	720.53	Joback Method
cpg	773.62	J/mol×K	749.11	Joback Method
cpg	789.63	J/mol×K	777.70	Joback Method
cpg	804.87	J/mol×K	806.29	Joback Method
cpg	819.36	J/mol×K	834.87	Joback Method
cpg	833.11	J/mol×K	863.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415257&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