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

Inchi: InChI=1S/C14H29NO2/c1-3-5-7-9-10-12-15-14(16)17-13-11-8-6-4-2/h3-13H2,1-2H3,(H,1

InchiKey: RONSWADFFUQVDH-UHFFFAOYSA-N

Formula: C14H29NO2

SMILES: CCCCCCCNC(=O)OCCCCCC

Mol. weight [g/mol]: 243.39

Physical Properties

Property code	Value	Unit	Source
gf	-77.53	kJ/mol	Joback Method
hf	-523.62	kJ/mol	Joback Method
hfus	39.90	kJ/mol	Joback Method
hvap	62.35	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.263		Crippen Method
mcvol	225.540	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	1821.00		NIST Webbook
rinpol	1821.00		NIST Webbook
tb	646.18	K	Joback Method
tc	817.40	K	Joback Method
tf	372.36	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.35	J/mol×K	646.18	Joback Method
cpg	644.05	J/mol×K	674.72	Joback Method
cpg	660.01	J/mol×K	703.25	Joback Method
cpg	675.25	J/mol×K	731.79	Joback Method
cpg	689.78	J/mol×K	760.33	Joback Method
cpg	703.63	J/mol×K	788.86	Joback Method
cpg	716.80	J/mol×K	817.40	Joback Method

Sources

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=U406710&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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