Carbonic acid, monoamide, N-ethyl-, decyl ester

Inchi: InChI=1S/C13H27NO2/c1-3-5-6-7-8-9-10-11-12-16-13(15)14-4-2/h3-12H2,1-2H3,(H,14,1

InchiKey: RSBLXFCWHMYOIN-UHFFFAOYSA-N

Formula: C13H27NO2

SMILES: CCCCCCCCCCOC(=O)NCC

Mol. weight [g/mol]: 229.36

Physical Properties

Property code	Value	Unit	Source
gf	-85.95	kJ/mol	Joback Method
hf	-502.98	kJ/mol	Joback Method
hfus	37.31	kJ/mol	Joback Method
hvap	60.12	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.873		Crippen Method
mcvol	211.450	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	623.30	K	Joback Method
tc	794.98	K	Joback Method
tf	361.09	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.38	J/mol×K	623.30	Joback Method
cpg	589.56	J/mol×K	651.91	Joback Method
cpg	605.06	J/mol×K	680.53	Joback Method
cpg	619.86	J/mol×K	709.14	Joback Method
cpg	634.00	J/mol×K	737.75	Joback Method
cpg	647.47	J/mol×K	766.37	Joback Method
cpg	660.30	J/mol×K	794.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415173&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