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

Inchi: InChI=1S/C17H35NO2/c1-3-5-7-9-10-11-12-13-15-18-17(19)20-16-14-8-6-4-2/h3-16H2,1

InchiKey: DUAHNCCLTCEGAV-UHFFFAOYSA-N

Formula: C17H35NO2

SMILES: CCCCCCCCCCNC(=O)OCCCCCC

Mol. weight [g/mol]: 285.47

Physical Properties

Property code	Value	Unit	Source
gf	-52.27	kJ/mol	Joback Method
hf	-585.54	kJ/mol	Joback Method
hfus	47.67	kJ/mol	Joback Method
hvap	69.03	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.434		Crippen Method
mcvol	267.810	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
rinpol	2127.00		NIST Webbook
rinpol	2127.00		NIST Webbook
tb	714.82	K	Joback Method
tc	887.21	K	Joback Method
tf	406.17	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.92	J/mol×K	714.82	Joback Method
cpg	814.96	J/mol×K	743.55	Joback Method
cpg	832.15	J/mol×K	772.28	Joback Method
cpg	848.52	J/mol×K	801.01	Joback Method
cpg	864.08	J/mol×K	829.74	Joback Method
cpg	878.85	J/mol×K	858.48	Joback Method
cpg	892.85	J/mol×K	887.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406707&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