Carbonic acid, monoamide, N-hept-2-yl-, hexyl ester

Inchi: InChI=1S/C14H29NO2/c1-4-6-8-10-12-17-14(16)15-13(3)11-9-7-5-2/h13H,4-12H2,1-3H3

InchiKey: YZSWAQDNAALBIZ-UHFFFAOYSA-N

Formula: C14H29NO2

SMILES: CCCCCCOC(=O)NC(C)CCCCC

Mol. weight [g/mol]: 243.39

Physical Properties

Property code	Value	Unit	Source
gf	-79.97	kJ/mol	Joback Method
hf	-528.90	kJ/mol	Joback Method
hfus	36.38	kJ/mol	Joback Method
hvap	61.96	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.262		Crippen Method
mcvol	225.540	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	1714.00		NIST Webbook
rinpol	1714.00		NIST Webbook
tb	645.74	K	Joback Method
tc	819.35	K	Joback Method
tf	357.36	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.76	J/mol×K	645.74	Joback Method
cpg	644.72	J/mol×K	674.68	Joback Method
cpg	660.93	J/mol×K	703.61	Joback Method
cpg	676.38	J/mol×K	732.55	Joback Method
cpg	691.11	J/mol×K	761.48	Joback Method
cpg	705.12	J/mol×K	790.42	Joback Method
cpg	718.42	J/mol×K	819.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406713&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