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

Inchi: InChI=1S/C11H23NO2/c1-3-5-6-7-8-9-12-11(13)14-10-4-2/h3-10H2,1-2H3,(H,12,13)
InchiKey: MJEQGJZWHVKFOZ-UHFFFAOYSA-N
Formula: C11H23NO2
SMILES: CCCCCCCNC(=O)OCCC
Mol. weight [g/mol]: 201.31

Physical Properties

Property code	Value	Unit	Source
gf	-102.79	kJ/mol	Joback Method
hf	-461.70	kJ/mol	Joback Method
hfus	32.13	kJ/mol	Joback Method
hvap	55.67	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.093		Crippen Method
mcvol	183.270	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	577.54	K	Joback Method
tc	751.09	K	Joback Method
tf	338.55	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.80	J/mol×K	577.54	Joback Method
cpg	484.82	J/mol×K	606.47	Joback Method
cpg	499.22	J/mol×K	635.39	Joback Method
cpg	513.00	J/mol×K	664.32	Joback Method
cpg	526.18	J/mol×K	693.24	Joback Method
cpg	538.76	J/mol×K	722.17	Joback Method
cpg	550.76	J/mol×K	751.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415252&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