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

Inchi: InChI=1S/C16H33NO2/c1-4-6-8-9-10-12-14-19-16(18)17-15(3)13-11-7-5-2/h15H,4-14H2

InchiKey: RZUPQBHXUGKNQT-UHFFFAOYSA-N

Formula: C16H33NO2

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

Mol. weight [g/mol]: 271.44

Physical Properties

Property code	Value	Unit	Source
gf	-63.13	kJ/mol	Joback Method
hf	-570.18	kJ/mol	Joback Method
hfus	41.56	kJ/mol	Joback Method
hvap	66.41	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.042		Crippen Method
mcvol	253.720	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook
tb	691.50	K	Joback Method
tc	864.93	K	Joback Method
tf	379.90	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.65	J/mol×K	691.50	Joback Method
cpg	757.48	J/mol×K	720.40	Joback Method
cpg	774.48	J/mol×K	749.31	Joback Method
cpg	790.66	J/mol×K	778.21	Joback Method
cpg	806.05	J/mol×K	807.12	Joback Method
cpg	820.67	J/mol×K	836.02	Joback Method
cpg	834.52	J/mol×K	864.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406446&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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