Carbonic acid, monoamide, N-pentyl-, menthyl ester

Inchi: InChI=1S/C16H31NO2/c1-5-6-7-10-17-16(18)19-15-11-13(4)8-9-14(15)12(2)3/h12-15H,5

InchiKey: NUNDBFKCSPKBBF-UHFFFAOYSA-N

Formula: C16H31NO2

SMILES: CCCCCNC(=O)OC1CC(C)CCC1C(C)C

Mol. weight [g/mol]: 269.42

Physical Properties

Property code	Value	Unit	Source
gf	-54.10	kJ/mol	Joback Method
hf	-556.54	kJ/mol	Joback Method
hfus	35.54	kJ/mol	Joback Method
hvap	66.22	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.364		Crippen Method
mcvol	242.860	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	2002.00		NIST Webbook
rinpol	2002.00		NIST Webbook
tb	701.71	K	Joback Method
tc	895.90	K	Joback Method
tf	378.80	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.32	J/mol×K	701.71	Joback Method
cpg	760.18	J/mol×K	734.08	Joback Method
cpg	779.85	J/mol×K	766.44	Joback Method
cpg	798.35	J/mol×K	798.81	Joback Method
cpg	815.70	J/mol×K	831.17	Joback Method
cpg	831.92	J/mol×K	863.54	Joback Method
cpg	847.01	J/mol×K	895.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415197&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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