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

Inchi: InChI=1S/C17H33NO2/c1-5-6-7-8-11-18-17(19)20-16-12-14(4)9-10-15(16)13(2)3/h13-16

InchiKey: YGEAFHAMAJEXBE-UHFFFAOYSA-N

Formula: C17H33NO2

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

Mol. weight [g/mol]: 283.45

Physical Properties

Property code	Value	Unit	Source
gf	-45.68	kJ/mol	Joback Method
hf	-577.18	kJ/mol	Joback Method
hfus	38.13	kJ/mol	Joback Method
hvap	68.45	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.754		Crippen Method
mcvol	256.950	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	724.59	K	Joback Method
tc	917.42	K	Joback Method
tf	390.07	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.08	J/mol×K	724.59	Joback Method
cpg	819.06	J/mol×K	756.73	Joback Method
cpg	838.82	J/mol×K	788.87	Joback Method
cpg	857.38	J/mol×K	821.01	Joback Method
cpg	874.77	J/mol×K	853.14	Joback Method
cpg	890.99	J/mol×K	885.28	Joback Method
cpg	906.07	J/mol×K	917.42	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=U415199&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