

Carbonic acid, monoamide, N-3-methylbutyl-, menthyl ester

Inchi:	InChI=1S/C16H31NO2/c1-11(2)8-9-17-16(18)19-15-10-13(5)6-7-14(15)12(3)4/h11-15H,6
InchiKey:	SCCXAJFKABEXQB-UHFFFAOYSA-N
Formula:	C16H31NO2
SMILES:	CC(C)CCNC(=O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]:	269.42

Physical Properties

Property code	Value	Unit	Source
gf	-56.54	kJ/mol	Joback Method
hf	-561.82	kJ/mol	Joback Method
hfus	32.01	kJ/mol	Joback Method
hvap	65.84	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.220		Crippen Method
mvol	242.860	ml/mol	McGowan Method
pc	1550.00	kPa	Joback Method
rinpol	1982.00		NIST Webbook
rinpol	1982.00		NIST Webbook
tb	701.27	K	Joback Method
tc	898.47	K	Joback Method
tf	363.80	K	Joback Method
vc	0.909	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.75	J/mol×K	701.27	Joback Method
cpg	760.96	J/mol×K	734.14	Joback Method
cpg	780.93	J/mol×K	767.00	Joback Method
cpg	799.69	J/mol×K	799.87	Joback Method
cpg	817.25	J/mol×K	832.74	Joback Method
cpg	833.63	J/mol×K	865.60	Joback Method
cpg	848.85	J/mol×K	898.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/116-431-4/Carbonic-acid-monoamide-N-3-methylbutyl-menthyl-ester.pdf>

Generated by Cheméo on 2024-04-30 03:17:02.751032646 +0000 UTC m=+16736271.671609957.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.