

Carbonic acid, neopentyl cyclohexylmethyl ester

Inchi:	InChI=1S/C13H24O3/c1-13(2,3)10-16-12(14)15-9-11-7-5-4-6-8-11/h11H,4-10H2,1-3H3
InchiKey:	JHYJFXWJFIIVJX-UHFFFAOYSA-N
Formula:	C13H24O3
SMILES:	CC(C)(C)COC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	228.33

Physical Properties

Property code	Value	Unit	Source
gf	-253.05	kJ/mol	Joback Method
hf	-643.10	kJ/mol	Joback Method
hfus	17.82	kJ/mol	Joback Method
hvap	55.23	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.766		Crippen Method
mcvol	196.480	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
tb	611.87	K	Joback Method
tc	817.77	K	Joback Method
tf	340.46	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.56	J/molxK	611.87	Joback Method
cpg	558.59	J/molxK	646.19	Joback Method
cpg	577.47	J/molxK	680.50	Joback Method
cpg	595.22	J/molxK	714.82	Joback Method
cpg	611.87	J/molxK	749.14	Joback Method
cpg	627.44	J/molxK	783.46	Joback Method
cpg	641.97	J/molxK	817.77	Joback Method
dvisc	0.0028479	Paxs	340.46	Joback Method

dvisc	0.0012503	Paxs	385.69	Joback Method
dvisc	0.0006525	Paxs	430.93	Joback Method
dvisc	0.0003853	Paxs	476.16	Joback Method
dvisc	0.0002493	Paxs	521.40	Joback Method
dvisc	0.0001729	Paxs	566.63	Joback Method
dvisc	0.0001266	Paxs	611.87	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=U357858&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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