

Carbonic acid, neopentyl 2-ethylhexyl ester

Inchi:	InChI=1S/C14H28O3/c1-6-8-9-12(7-2)10-16-13(15)17-11-14(3,4)5/h12H,6-11H2,1-5H3
InchiKey:	LGERJXMQUXDYGA-UHFFFAOYSA-N
Formula:	C14H28O3
SMILES:	CCCCC(CC)COC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	244.37

Physical Properties

Property code	Value	Unit	Source
gf	-271.52	kJ/mol	Joback Method
hf	-723.34	kJ/mol	Joback Method
hfus	25.05	kJ/mol	Joback Method
hvap	56.64	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.402		Crippen Method
mcvol	221.430	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpola	1483.00		NIST Webbook
tb	614.76	K	Joback Method
tc	793.00	K	Joback Method
tf	329.35	K	Joback Method
vc	0.845	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.56	J/molxK	614.76	Joback Method
cpg	617.19	J/molxK	644.47	Joback Method
cpg	634.01	J/molxK	674.17	Joback Method
cpg	650.02	J/molxK	703.88	Joback Method
cpg	665.25	J/molxK	733.59	Joback Method
cpg	679.72	J/molxK	763.30	Joback Method
cpg	693.44	J/molxK	793.00	Joback Method
dvisc	0.0029057	Paxs	329.35	Joback Method
dvisc	0.0011595	Paxs	376.92	Joback Method

dvisc	0.0005685	Paxs	424.49	Joback Method
dvisc	0.0003218	Paxs	472.06	Joback Method
dvisc	0.0002021	Paxs	519.62	Joback Method
dvisc	0.0001373	Paxs	567.19	Joback Method
dvisc	0.0000990	Paxs	614.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U357857&Units=SI

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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