

Carbonic acid, dihexyl ester

Other names:	Dihexyl carbonate (n-C6H13)OC(O)O(n-C6H13) Di-n-hexyl carbonate
Inchi:	InChI=1S/C13H26O3/c1-3-5-7-9-11-15-13(14)16-12-10-8-6-4-2/h3-12H2,1-2H3
InchiKey:	OKQDSOXFNBWWJL-UHFFFAOYSA-N
Formula:	C13H26O3
SMILES:	CCCCCOC(=O)OCCCCC
Mol. weight [g/mol]:	230.34
CAS:	7523-15-1

Physical Properties

Property code	Value	Unit	Source
gf	-280.34	kJ/mol	Joback Method
hf	-688.67	kJ/mol	Joback Method
hfus	33.40	kJ/mol	Joback Method
hvap	56.10	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.300		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
tb	595.55	K	Joback Method
tc	764.22	K	Joback Method
tf	330.66	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.50	J/mol×K	595.55	Joback Method
cpg	617.73	J/mol×K	736.11	Joback Method
cpg	604.13	J/mol×K	708.00	Joback Method
cpg	589.90	J/mol×K	679.89	Joback Method
cpg	575.06	J/mol×K	651.77	Joback Method
cpg	559.59	J/mol×K	623.66	Joback Method

cpg	630.73	J/mol×K	764.22	Joback Method
dvisc	0.0001347	Pa×s	595.55	Joback Method
dvisc	0.0001769	Pa×s	551.40	Joback Method
dvisc	0.0002435	Pa×s	507.25	Joback Method
dvisc	0.0003562	Pa×s	463.10	Joback Method
dvisc	0.0005647	Pa×s	418.96	Joback Method
dvisc	0.0009978	Pa×s	374.81	Joback Method
dvisc	0.0020526	Pa×s	330.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7523151&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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