Carbonic acid, neopentyl 2-pentyl ester

Inchi: InChI=1S/C11H22O3/c1-6-7-9(2)14-10(12)13-8-11(3,4)5/h9H,6-8H2,1-5H3
InchiKey: IPTUBJGOJROINE-UHFFFAOYSA-N
Formula: C11H22O3
SMILES: CCCC(C)OC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 202.29

Physical Properties

Property code	Value	Unit	Source
gf	-296.78	kJ/mol	Joback Method
hf	-661.42	kJ/mol	Joback Method
hfus	17.28	kJ/mol	Joback Method
hvap	49.96	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.374		Crippen Method
mcvol	179.160	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1190.00		NIST Webbook
rinpol	1190.00		NIST Webbook
tb	546.12	K	Joback Method
tc	729.24	K	Joback Method
tf	295.54	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.55	J/mol×K	546.12	Joback Method
cpg	461.52	J/mol×K	576.64	Joback Method
cpg	476.78	J/mol×K	607.16	Joback Method
cpg	491.33	J/mol×K	637.68	Joback Method
cpg	505.20	J/mol×K	668.20	Joback Method
cpg	518.39	J/mol×K	698.72	Joback Method
cpg	530.91	J/mol×K	729.24	Joback Method
dvisc	0.0038637	Pa×s	295.54	Joback Method

dvisc	0.0015930	Pa×s	337.30	Joback Method
dvisc	0.0007983	Pa×s	379.07	Joback Method
dvisc	0.0004589	Pa×s	420.83	Joback Method
dvisc	0.0002915	Pa×s	462.59	Joback Method
dvisc	0.0001996	Pa×s	504.36	Joback Method
dvisc	0.0001449	Pa×s	546.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357854&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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