

Carbonic acid, neopentyl cyclohexyl ester

Inchi:	InChI=1S/C12H22O3/c1-12(2,3)9-14-11(13)15-10-7-5-4-6-8-10/h10H,4-9H2,1-3H3
InchiKey:	DZJZBIPEXUAHJX-UHFFFAOYSA-N
Formula:	C12H22O3
SMILES:	CC(C)(C)COC(=O)OC1CCCCC1
Mol. weight [g/mol]:	214.30

Physical Properties

Property code	Value	Unit	Source
gf	-261.47	kJ/mol	Joback Method
hf	-622.46	kJ/mol	Joback Method
hfus	15.23	kJ/mol	Joback Method
hvap	53.00	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.518		Crippen Method
mvol	182.390	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	1408.00		NIST Webbook
tb	588.99	K	Joback Method
tc	798.14	K	Joback Method
tf	329.19	K	Joback Method
vc	0.671	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.95	J/molxK	588.99	Joback Method
cpg	505.61	J/molxK	623.85	Joback Method
cpg	524.15	J/molxK	658.71	Joback Method
cpg	541.57	J/molxK	693.56	Joback Method
cpg	557.92	J/molxK	728.42	Joback Method
cpg	573.21	J/molxK	763.28	Joback Method
cpg	587.47	J/molxK	798.14	Joback Method
dvisc	0.0031157	Paxs	329.19	Joback Method
dvisc	0.0013852	Paxs	372.49	Joback Method

dvisc	0.0007291	Paxs	415.79	Joback Method
dvisc	0.0004332	Paxs	459.09	Joback Method
dvisc	0.0002815	Paxs	502.39	Joback Method
dvisc	0.0001959	Paxs	545.69	Joback Method
dvisc	0.0001438	Paxs	588.99	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=U357855&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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