

Carbonic acid, isobutyl 2-pentyl ester

Inchi:	InChI=1S/C10H20O3/c1-5-6-9(4)13-10(11)12-7-8(2)3/h8-9H,5-7H2,1-4H3
InchiKey:	BNBBJRKBAZHRAB-UHFFFAOYSA-N
Formula:	C10H20O3
SMILES:	CCCC(C)OC(=O)OCC(C)C
Mol. weight [g/mol]:	188.26

Physical Properties

Property code	Value	Unit	Source
gf	-310.48	kJ/mol	Joback Method
hf	-637.31	kJ/mol	Joback Method
hfus	18.59	kJ/mol	Joback Method
hvap	48.64	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.984		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1161.00		NIST Webbook
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tb	526.03	K	Joback Method
tc	704.59	K	Joback Method
tf	266.85	K	Joback Method
vc	0.625	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.72	J/molxK	526.03	Joback Method
cpg	409.35	J/molxK	555.79	Joback Method
cpg	423.43	J/molxK	585.55	Joback Method
cpg	436.98	J/molxK	615.31	Joback Method
cpg	449.98	J/molxK	645.07	Joback Method
cpg	462.43	J/molxK	674.83	Joback Method
cpg	474.34	J/molxK	704.59	Joback Method
dvisc	0.0046442	Paxs	266.85	Joback Method

dvisc	0.0017975	Paxs	310.05	Joback Method
dvisc	0.0008775	Paxs	353.24	Joback Method
dvisc	0.0005009	Paxs	396.44	Joback Method
dvisc	0.0003192	Paxs	439.64	Joback Method
dvisc	0.0002205	Paxs	482.83	Joback Method
dvisc	0.0001618	Paxs	526.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357825&Units=SI
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

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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