

Carbonic acid, isobutyl cyclohexylmethyl ester

Inchi:	InChI=1S/C12H22O3/c1-10(2)8-14-12(13)15-9-11-6-4-3-5-7-11/h10-11H,3-9H2,1-2H3
InchiKey:	FJMBJSZKZAOJSK-UHFFFAOYSA-N
Formula:	C12H22O3
SMILES:	CC(C)COC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	214.30

Physical Properties

Property code	Value	Unit	Source
gf	-266.75	kJ/mol	Joback Method
hf	-618.99	kJ/mol	Joback Method
hfus	19.12	kJ/mol	Joback Method
hvap	53.91	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	3.376		Crippen Method
mvol	182.390	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1486.00		NIST Webbook
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tb	591.78	K	Joback Method
tc	793.39	K	Joback Method
tf	311.77	K	Joback Method
vc	0.676	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.43	J/molxK	591.78	Joback Method
cpg	502.48	J/molxK	625.38	Joback Method
cpg	520.55	J/molxK	658.98	Joback Method
cpg	537.66	J/molxK	692.58	Joback Method
cpg	553.80	J/molxK	726.18	Joback Method
cpg	568.98	J/molxK	759.79	Joback Method
cpg	583.21	J/molxK	793.39	Joback Method
dvisc	0.0035818	Paxs	311.77	Joback Method

dvisc	0.0014946	Paxs	358.44	Joback Method
dvisc	0.0007628	Paxs	405.11	Joback Method
dvisc	0.0004474	Paxs	451.77	Joback Method
dvisc	0.0002899	Paxs	498.44	Joback Method
dvisc	0.0002024	Paxs	545.11	Joback Method
dvisc	0.0001495	Paxs	591.78	Joback Method

Sources

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=U357830&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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