

Carbonic acid, 2-ethylhexyl isobutyl ester

Inchi:	InChI=1S/C13H26O3/c1-5-7-8-12(6-2)10-16-13(14)15-9-11(3)4/h11-12H,5-10H2,1-4H3
InchiKey:	NPSPGHZMMKOHJM-UHFFFAOYSA-N
Formula:	C13H26O3
SMILES:	CCCCC(CC)COC(=O)OCC(C)C
Mol. weight [g/mol]:	230.34

Physical Properties

Property code	Value	Unit	Source
gf	-285.22	kJ/mol	Joback Method
hf	-699.23	kJ/mol	Joback Method
hfus	26.36	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	4.012		Crippen Method
mvol	207.340	ml/mol	McGowan Method
pc	1706.12	kPa	Joback Method
rinpol	1427.00		NIST Webbook
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tb	594.67	K	Joback Method
tc	768.89	K	Joback Method
tf	300.66	K	Joback Method
vc	0.793	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.19	J/molxK	594.67	Joback Method
cpg	560.91	J/molxK	623.71	Joback Method
cpg	576.94	J/molxK	652.74	Joback Method
cpg	592.30	J/molxK	681.78	Joback Method
cpg	606.98	J/molxK	710.81	Joback Method
cpg	620.98	J/molxK	739.85	Joback Method
cpg	634.32	J/molxK	768.89	Joback Method
dvisc	0.0037201	Paxs	300.66	Joback Method

dvisc	0.0013975	Paxs	349.66	Joback Method
dvisc	0.0006678	Paxs	398.66	Joback Method
dvisc	0.0003751	Paxs	447.67	Joback Method
dvisc	0.0002361	Paxs	496.67	Joback Method
dvisc	0.0001615	Paxs	545.67	Joback Method
dvisc	0.0001176	Paxs	594.67	Joback Method

Sources

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=U383133&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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