

Carbonic acid, 2-methoxyethyl 2-ethylhexyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C12H24O4/c1-4-6-7-11(5-2)10-16-12(13)15-9-8-14-3/h11H,4-10H2,1-3H3

RIGSYMLFBGNOPA-UHFFFAOYSA-N

C12H24O4

CCCCC(CC)COC(=O)OCCOC

232.32

Physical Properties

Property code	Value	Unit	Source
gf	-396.20	kJ/mol	Joback Method
hf	-805.53	kJ/mol	Joback Method
hfus	28.48	kJ/mol	Joback Method
hvap	55.89	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	3.002		Crippen Method
mcvol	199.120	ml/mol	McGowan Method
pc	1810.77	kPa	Joback Method
rinpol	1525.00		NIST Webbook
tb	594.65	K	Joback Method
tc	766.74	K	Joback Method
tf	326.62	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.38	J/mol×K	594.65	Joback Method
cpg	535.96	J/mol×K	623.33	Joback Method
cpg	550.96	J/mol×K	652.01	Joback Method
cpg	565.35	J/mol×K	680.69	Joback Method
cpg	579.14	J/mol×K	709.38	Joback Method
cpg	592.33	J/mol×K	738.06	Joback Method
cpg	604.89	J/mol×K	766.74	Joback Method
dvisc	0.0019812	Pa×s	326.62	Joback Method
dvisc	0.0009172	Pa×s	371.29	Joback Method

dvisc	0.0005010	Pa×s	415.96	Joback Method
dvisc	0.0003077	Pa×s	460.63	Joback Method
dvisc	0.0002060	Pa×s	505.31	Joback Method
dvisc	0.0001472	Pa×s	549.98	Joback Method
dvisc	0.0001107	Pa×s	594.65	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357869&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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