Carbonic acid, butyl 2-ethylhexyl ester

Inchi: InChI=1S/C13H26O3/c1-4-7-9-12(6-3)11-16-13(14)15-10-8-5-2/h12H,4-11H2,1-3H3
InchiKey: DGCRQNVSIHHFIC-UHFFFAOYSA-N
Formula: C13H26O3
SMILES: CCCCOC(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 230.34

Physical Properties

Property code	Value	Unit	Source
gf	-282.78	kJ/mol	Joback Method
hf	-693.95	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	55.71	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	4.156		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
tb	595.11	K	Joback Method
tc	766.49	K	Joback Method
tf	315.66	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.85	J/mol×K	595.11	Joback Method
cpg	560.25	J/mol×K	623.67	Joback Method
cpg	575.99	J/mol×K	652.24	Joback Method
cpg	591.08	J/mol×K	680.80	Joback Method
cpg	605.53	J/mol×K	709.37	Joback Method
cpg	619.34	J/mol×K	737.93	Joback Method
cpg	632.50	J/mol×K	766.49	Joback Method
dvisc	0.0027073	Pa×s	315.66	Joback Method

dvisc	0.0011685	Pa×s	362.23	Joback Method
dvisc	0.0006108	Pa×s	408.81	Joback Method
dvisc	0.0003646	Pa×s	455.38	Joback Method
dvisc	0.0002395	Pa×s	501.96	Joback Method
dvisc	0.0001689	Pa×s	548.54	Joback Method
dvisc	0.0001259	Pa×s	595.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357844&Units=SI
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

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