Carbonic acid, butyl 4-chlorophenyl ester

Inchi: InChI=1S/C11H13ClO3/c1-2-3-8-14-11(13)15-10-6-4-9(12)5-7-10/h4-7H,2-3,8H2,1H3
InchiKey: FUBRDBALXONBRA-UHFFFAOYSA-N
Formula: C11H13ClO3
SMILES: CCCCOC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 228.67

Physical Properties

Property code	Value	Unit	Source
gf	-206.33	kJ/mol	Joback Method
hf	-438.07	kJ/mol	Joback Method
hfus	26.07	kJ/mol	Joback Method
hvap	58.97	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.655		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	1610.00		NIST Webbook
tb	618.88	K	Joback Method
tc	830.85	K	Joback Method
tf	376.98	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.18	J/mol×K	618.88	Joback Method
cpg	455.20	J/mol×K	795.52	Joback Method
cpg	445.07	J/mol×K	760.19	Joback Method
cpg	434.21	J/mol×K	724.87	Joback Method
cpg	422.61	J/mol×K	689.54	Joback Method
cpg	410.26	J/mol×K	654.21	Joback Method
cpg	464.60	J/mol×K	830.85	Joback Method
dvisc	0.0001522	Pa×s	618.88	Joback Method
dvisc	0.0001905	Pa×s	578.56	Joback Method

dvisc	0.0002464	Pa×s	538.25	Joback Method
dvisc	0.0003324	Pa×s	497.93	Joback Method
dvisc	0.0004728	Pa×s	457.61	Joback Method
dvisc	0.0007196	Pa×s	417.30	Joback Method
dvisc	0.0011984	Pa×s	376.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357847&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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