Carbonic acid, butyl 3,4-dichlorophenyl ester

Inchi: InChI=1S/C11H12Cl2O3/c1-2-3-6-15-11(14)16-8-4-5-9(12)10(13)7-8/h4-5,7H,2-3,6H2,1H
InchiKey: SUZWMLPWLFCULQ-UHFFFAOYSA-N
Formula: C11H12Cl2O3
SMILES: CCCCOC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 263.12

Physical Properties

Property code	Value	Unit	Source
gf	-227.89	kJ/mol	Joback Method
hf	-465.28	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	64.02	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.309		Crippen Method
mcvol	179.880	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1795.00		NIST Webbook
tb	661.29	K	Joback Method
tc	877.62	K	Joback Method
tf	419.42	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.93	J/mol×K	661.29	Joback Method
cpg	473.70	J/mol×K	841.57	Joback Method
cpg	464.62	J/mol×K	805.51	Joback Method
cpg	454.81	J/mol×K	769.46	Joback Method
cpg	444.25	J/mol×K	733.40	Joback Method
cpg	432.96	J/mol×K	697.35	Joback Method
cpg	482.04	J/mol×K	877.62	Joback Method
dvisc	0.0001399	Pa×s	661.29	Joback Method
dvisc	0.0001721	Pa×s	620.98	Joback Method

dvisc	0.0002179	Pa×s	580.67	Joback Method
dvisc	0.0002858	Pa×s	540.36	Joback Method
dvisc	0.0003915	Pa×s	500.04	Joback Method
dvisc	0.0005668	Pa×s	459.73	Joback Method
dvisc	0.0008811	Pa×s	419.42	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U357851&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