Trichloroacetic acid butyl ester

Other names:	Butyl trichloroacetate
	Acetic acid, trichloro-, butyl ester
	n-Butyl trichloroacetate
Inchi:	InChI=1S/C6H9Cl3O2/c1-2-3-4-11-5(10)6(7,8)9/h2-4H2,1H3
InchiKey:	SECVZLDDYUWJAC-UHFFFAOYSA-N
Formula:	C6H9Cl3O2
SMILES:	CCCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	219.49
CAS:	3657-07-6

Physical Properties

Property code	Value	Unit	Source
chl	-3168.20 ± 4.20	kJ/mol	NIST Webbook
chl	-3161.00	kJ/mol	NIST Webbook
gf	-267.23	kJ/mol	Joback Method
hf	-492.90 ± 9.60	kJ/mol	NIST Webbook
hfl	-546.40 ± 8.40	kJ/mol	NIST Webbook
hfus	19.26	kJ/mol	Joback Method
hvap	53.60 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.76		Crippen Method
logp	2.700		Crippen Method
mcvol	139.560	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1144.50		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1148.00		NIST Webbook
ripol	1542.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1554.00		NIST Webbook

ripol	1550.00		NIST Webbook
ripol	1542.00		NIST Webbook
tb	522.03	K	Joback Method
tc	729.87	K	Joback Method
tf	321.72	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.69	J/mol×K	522.03	Joback Method
cpg	317.49	J/mol×K	695.23	Joback Method
cpg	310.22	J/mol×K	660.59	Joback Method
cpg	302.43	J/mol×K	625.95	Joback Method
cpg	294.09	J/mol×K	591.31	Joback Method
cpg	285.19	J/mol×K	556.67	Joback Method
cpg	324.26	J/mol×K	729.87	Joback Method
dvisc	0.0002830	Pa×s	522.03	Joback Method
dvisc	0.0003676	Pa×s	488.64	Joback Method
dvisc	0.0004962	Pa×s	455.26	Joback Method
dvisc	0.0007022	Pa×s	421.88	Joback Method
dvisc	0.0010550	Pa×s	388.49	Joback Method
dvisc	0.0017110	Pa×s	355.11	Joback Method
dvisc	0.0030680	Pa×s	321.72	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3657076&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

chl: Standard liquid enthalpy of combustion

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume