

Dichloroacetic acid butyl ester

Other names:	Acetic acid, dichloro-, butyl ester Butyl dichloroacetate 1-Butanol, dichloroacetate n-Butyl dichloroacetate
Inchi:	InChI=1S/C6H10Cl2O2/c1-2-3-4-10-6(9)5(7)8/h5H,2-4H2,1H3
InchiKey:	MASXONVJEAXEIV-UHFFFAOYSA-N
Formula:	C6H10Cl2O2
SMILES:	CCCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]:	185.05
CAS:	29003-73-4

Physical Properties

Property code	Value	Unit	Source
chl	-3279.00	kJ/mol	NIST Webbook
chl	-3283.30 ± 4.20	kJ/mol	NIST Webbook
gf	-260.58	kJ/mol	Joback Method
hf	-497.90 ± 9.60	kJ/mol	NIST Webbook
hfl	-550.20 ± 8.40	kJ/mol	NIST Webbook
hfus	18.95	kJ/mol	Joback Method
hvap	52.30 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.11		Crippen Method
logp	2.133		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1070.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1069.80		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1061.00		NIST Webbook
ripol	1542.00		NIST Webbook
ripol	1575.00		NIST Webbook
ripol	1559.00		NIST Webbook

ripol	1554.00		NIST Webbook
ripol	1542.00		NIST Webbook
ripol	1562.00		NIST Webbook
tb	487.39	K	Joback Method
tc	681.93	K	Joback Method
tf	274.38	K	Joback Method
vc	0.487	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.20	J/molxK	487.39	Joback Method
cpg	292.82	J/molxK	649.50	Joback Method
cpg	284.91	J/molxK	617.08	Joback Method
cpg	276.59	J/molxK	584.66	Joback Method
cpg	267.87	J/molxK	552.24	Joback Method
cpg	258.74	J/molxK	519.81	Joback Method
cpg	300.33	J/molxK	681.93	Joback Method
dvisc	0.0002910	Paxs	487.39	Joback Method
dvisc	0.0003781	Paxs	451.89	Joback Method
dvisc	0.0005137	Paxs	416.39	Joback Method
dvisc	0.0007390	Paxs	380.88	Joback Method
dvisc	0.0011455	Paxs	345.38	Joback Method
dvisc	0.0019631	Paxs	309.88	Joback Method
dvisc	0.0038678	Paxs	274.38	Joback Method

Sources

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=C29003734&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/38-004-5/Dichloroacetic-acid-butyl-ester.pdf>

Generated by Cheméo on 2024-04-23 11:53:53.165770848 +0000 UTC m=+16162482.086348161.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.