3-Buten-1-ol, dichloroacetate

Inchi: InChI=1S/C6H8Cl2O2/c1-2-3-4-10-6(9)5(7)8/h2,5H,1,3-4H2
InchiKey: UHMUQRQTBDMYQV-UHFFFAOYSA-N
Formula: C6H8Cl2O2
SMILES: C=CCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 183.03

Physical Properties

Property code	Value	Unit	Source
gf	-172.74	kJ/mol	Joback Method
hf	-323.30	kJ/mol	Joback Method
hfus	17.67	kJ/mol	Joback Method
hvap	45.82	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.909		Crippen Method
mcvol	123.020	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1042.00		NIST Webbook
rinpol	1042.00		NIST Webbook
ripol	1576.00		NIST Webbook
tb	484.07	K	Joback Method
tc	682.73	K	Joback Method
tf	272.62	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.13	J/mol×K	484.07	Joback Method
cpg	240.92	J/mol×K	517.18	Joback Method
cpg	249.29	J/mol×K	550.29	Joback Method
cpg	257.25	J/mol×K	583.40	Joback Method
cpg	264.80	J/mol×K	616.51	Joback Method
cpg	271.96	J/mol×K	649.62	Joback Method
cpg	278.72	J/mol×K	682.73	Joback Method

dvisc	0.0035892	Pa×s	272.62	Joback Method
dvisc	0.0018651	Pa×s	307.86	Joback Method
dvisc	0.0011087	Pa×s	343.10	Joback Method
dvisc	0.0007261	Pa×s	378.35	Joback Method
dvisc	0.0005111	Pa×s	413.59	Joback Method
dvisc	0.0003802	Pa×s	448.83	Joback Method
dvisc	0.0002952	Pa×s	484.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26439&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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