

6-chlorooctyl dichloroacetate

Other names:	1-Octanol, 6-chloro, dichloroacetate
Inchi:	InChI=1S/C10H17Cl3O2/c1-2-8(11)6-4-3-5-7-15-10(14)9(12)13/h8-9H,2-7H2,1H3
InchiKey:	AKBOYQGLIOIBTO-UHFFFAOYSA-N
Formula:	C10H17Cl3O2
SMILES:	CCC(Cl)CCCCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]:	275.60

Physical Properties

Property code	Value	Unit	Source
gf	-241.27	kJ/mol	Joback Method
hf	-552.31	kJ/mol	Joback Method
hfus	29.99	kJ/mol	Joback Method
hvap	59.39	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.911		Crippen Method
mcvol	195.920	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1678.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1704.00		NIST Webbook
ripol	2391.00		NIST Webbook
ripol	2403.00		NIST Webbook
ripol	2372.00		NIST Webbook
tb	615.90	K	Joback Method
tc	809.16	K	Joback Method
tf	334.38	K	Joback Method
vc	0.754	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.66	J/mol×K	615.90	Joback Method
cpg	468.53	J/mol×K	648.11	Joback Method

cpg	480.73	J/molxK	680.32	Joback Method
cpg	492.28	J/molxK	712.53	Joback Method
cpg	503.19	J/molxK	744.74	Joback Method
cpg	513.48	J/molxK	776.95	Joback Method
cpg	523.15	J/molxK	809.16	Joback Method
dvisc	0.0033761	Paxs	334.38	Joback Method
dvisc	0.0014970	Paxs	381.30	Joback Method
dvisc	0.0007933	Paxs	428.22	Joback Method
dvisc	0.0004765	Paxs	475.14	Joback Method
dvisc	0.0003137	Paxs	522.06	Joback Method
dvisc	0.0002213	Paxs	568.98	Joback Method
dvisc	0.0001646	Paxs	615.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R112248&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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