

Octyl 3-chlorobutanoate

Other names:	Butanoic acid, 3-chloro, octyl ester
Inchi:	InChI=1S/C12H23ClO2/c1-3-4-5-6-7-8-9-15-12(14)10-11(2)13/h11H,3-10H2,1-2H3
InchiKey:	KGTJTJMGWKRVOB-UHFFFAOYSA-N
Formula:	C12H23ClO2
SMILES:	CCCCCCCCOC(=O)CC(C)Cl
Mol. weight [g/mol]:	234.76

Physical Properties

Property code	Value	Unit	Source
gf	-198.13	kJ/mol	Joback Method
hf	-556.83	kJ/mol	Joback Method
hfus	30.30	kJ/mol	Joback Method
hvap	55.46	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.907		Crippen Method
mcvol	199.620	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1531.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1547.00		NIST Webbook
tb	587.24	K	Joback Method
tc	764.85	K	Joback Method
tf	312.08	K	Joback Method
vc	0.774	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.78	J/mol×K	587.24	Joback Method

cpg	566.97	J/molxK	735.25	Joback Method
cpg	554.22	J/molxK	705.64	Joback Method
cpg	540.84	J/molxK	676.04	Joback Method
cpg	526.82	J/molxK	646.44	Joback Method
cpg	512.13	J/molxK	616.84	Joback Method
cpg	579.10	J/molxK	764.85	Joback Method
dvisc	0.0001665	Paxs	587.24	Joback Method
dvisc	0.0002228	Paxs	541.38	Joback Method
dvisc	0.0003146	Paxs	495.52	Joback Method
dvisc	0.0004765	Paxs	449.66	Joback Method
dvisc	0.0007932	Paxs	403.80	Joback Method
dvisc	0.0015046	Paxs	357.94	Joback Method
dvisc	0.0034450	Paxs	312.08	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=R28376&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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