

Formic acid, 8-chlorooctyl ester

Inchi:	InChI=1S/C9H17ClO2/c10-7-5-3-1-2-4-6-8-12-9-11/h9H,1-8H2
InchiKey:	ZTOVWAJPELYHBS-UHFFFAOYSA-N
Formula:	C9H17ClO2
SMILES:	O=COCCCCCCCCCI
Mol. weight [g/mol]:	192.68

Physical Properties

Property code	Value	Unit	Source
gf	-191.55	kJ/mol	Joback Method
hf	-462.63	kJ/mol	Joback Method
hfus	26.74	kJ/mol	Joback Method
hvap	49.14	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.739		Crippen Method
mvol	157.350	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1420.00		NIST Webbook
tb	513.83	K	Joback Method
tc	688.78	K	Joback Method
tf	285.34	K	Joback Method
vc	0.624	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.99	J/molxK	513.83	Joback Method
cpg	410.53	J/molxK	659.62	Joback Method
cpg	399.98	J/molxK	630.47	Joback Method
cpg	388.96	J/molxK	601.31	Joback Method
cpg	377.46	J/molxK	572.15	Joback Method
cpg	365.47	J/molxK	542.99	Joback Method
cpg	420.62	J/molxK	688.78	Joback Method
dvisc	0.0002622	Paxs	513.83	Joback Method
dvisc	0.0003387	Paxs	475.75	Joback Method

dvisc	0.0004575	Paxs	437.67	Joback Method
dvisc	0.0006543	Paxs	399.58	Joback Method
dvisc	0.0010093	Paxs	361.50	Joback Method
dvisc	0.0017241	Paxs	323.42	Joback Method
dvisc	0.0033977	Paxs	285.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U367928&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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