Chloroacetic acid, 6-chlorohexyl ester

Other names: 1-Hexanol, 6-chloro, chloroacetate
6-chlorohexyl chloroacetate
Inchi: InChI=1S/C8H14Cl2O2/c9-5-3-1-2-4-6-12-8(11)7-10/h1-7H2
InchiKey: VNGMYNDYUJRSGC-UHFFFAOYSA-N
Formula: C8H14Cl2O2
SMILES: O=C(CCl)OCCCCCCCl
Mol. weight [g/mol]: 213.10

Physical Properties

Property code	Value	Unit	Source
hf	-561.87	kJ/mol	Cheméo Relay (1.0)
hfus	29.24	kJ/mol	Joback Method
hvap	64.53	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.16		Cheméo Relay (1.0)
logp	2.568		Crippen Method
mcvol	155.500	ml/mol	McGowan Method
rinpol	1470.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1465.00		NIST Webbook
ripol	2211.00		NIST Webbook
ripol	2232.00		NIST Webbook
ripol	2226.00		NIST Webbook
ripol	2211.00		NIST Webbook
tb	523.51	K	Cheméo Relay (1.0)
tf	268.14	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K

Coeff. A	4.68070e+01
Coeff. B	7.22600e-01
Coeff. C	-3.57600e-04
Coeff. D	4.49000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.18272e+01
Coeff. B	1.79608e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	282.09
Temperature range (K), max.	489.31

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U330855&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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