

trichloromethyl carbonochloridate

Inchi: InChI=1S/C2Cl4O2/c3-1(7)8-2(4,5)6
InchiKey: HCUYBXPSSCRKRF-UHFFFAOYSA-N
Formula: C2Cl4O2
SMILES: O=C(Cl)OC(Cl)(Cl)Cl
Mol. weight [g/mol]: 197.83
CAS: 503-38-8

Physical Properties

Property code	Value	Unit	Source
hf	-456.19	kJ/mol	Cheméo Relay (1.0)
hfus	14.68	kJ/mol	Joback Method
ie	11.29	eV	Cheméo Relay (1.0)
logp	2.690		Crippen Method
mcvol	95.440	ml/mol	McGowan Method
tb	414.34	K	Cheméo Relay (1.0)
tf	216.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

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	5.35700e+01
Coeff. B	2.92000e-01
Coeff. C	-2.43800e-04
Coeff. D	6.34000e-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	$Y = \exp(A + B/T + C \cdot \ln(T) + D \cdot T^E)$
Y unit	Pa·s
Coeff. A	-1.18296e+01
Coeff. B	1.81430e+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.	216.15
Temperature range (K), max.	471.60

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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