METHYL 2,2,3,3-TETRACHLORO-PROPANOATE

Inchi: InChI=1S/C4H4Cl4O2/c1-10-3(9)4(7,8)2(5)6/h2H,1H3
InchiKey: UQYYMXYJSOOLLA-UHFFFAOYSA-N
Formula: C4H4Cl4O2
SMILES: COC(=O)C(Cl)(Cl)C(Cl)Cl
Mol. weight [g/mol]: 225.89

Physical Properties

Property code	Value	Unit	Source
hf	-476.53	kJ/mol	Cheméo Relay (1.0)
hfus	14.75	kJ/mol	Joback Method
hvap	60.68	kJ/mol	Cheméo Relay (1.0)
ie	11.13	eV	Cheméo Relay (1.0)
logp	2.137		Crippen Method
mcvol	123.620	ml/mol	McGowan Method
rinpol	1156.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1156.00		NIST Webbook
tb	475.15	K	Cheméo Relay (1.0)
tf	263.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.59	J/mol×K	513.26	Joback Method
cpg	222.27	J/mol×K	550.74	Joback Method
cpg	228.42	J/mol×K	588.22	Joback Method
cpg	234.07	J/mol×K	625.69	Joback Method
cpg	239.23	J/mol×K	663.17	Joback Method
cpg	243.95	J/mol×K	700.65	Joback Method
cpg	248.23	J/mol×K	738.13	Joback Method
dvisc	0.0038064	Pa×s	314.10	Joback Method
dvisc	0.0020592	Pa×s	347.29	Joback Method

dvisc	0.0012400	Pa×s	380.49	Joback Method
dvisc	0.0008101	Pa×s	413.68	Joback Method
dvisc	0.0005637	Pa×s	446.87	Joback Method
dvisc	0.0004125	Pa×s	480.07	Joback Method
dvisc	0.0003143	Pa×s	513.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20618057&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):	
Cheméo Relay (1.0, beta):	

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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point