2,2,2-Trichloroethyl eicosanoate

Inchi: InChI=1S/C22H41Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21(26)27-20
InchiKey: VJMDNNNSMGFIAL-UHFFFAOYSA-N
Formula: C22H41Cl3O2
SMILES: CCCCCCCCCCCCCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 443.92

Physical Properties

Property code	Value	Unit	Source
gf	-132.51	kJ/mol	Joback Method
hf	-798.18	kJ/mol	Joback Method
hfus	60.70	kJ/mol	Joback Method
hvap	85.58	kJ/mol	Joback Method
log10ws	-9.46		Crippen Method
logp	8.941		Crippen Method
mcvol	365.000	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinpol	2785.00		NIST Webbook
rinpol	2776.00		NIST Webbook
ripol	3172.00		NIST Webbook
ripol	3192.00		NIST Webbook
ripol	3191.00		NIST Webbook
ripol	3179.00		NIST Webbook
tb	888.11	K	Joback Method
tc	1087.65	K	Joback Method
tf	502.04	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1131.77	J/mol×K	888.11	Joback Method
cpg	1211.59	J/mol×K	1054.39	Joback Method
cpg	1197.52	J/mol×K	1021.14	Joback Method
cpg	1182.57	J/mol×K	987.88	Joback Method

cpg	1166.67	J/mol×K	954.62	Joback Method
cpg	1149.76	J/mol×K	921.37	Joback Method
cpg	1224.82	J/mol×K	1087.65	Joback Method
dvisc	0.0000267	Pa×s	888.11	Joback Method
dvisc	0.0000363	Pa×s	823.77	Joback Method
dvisc	0.0000521	Pa×s	759.42	Joback Method
dvisc	0.0000799	Pa×s	695.08	Joback Method
dvisc	0.0001336	Pa×s	630.73	Joback Method
dvisc	0.0002512	Pa×s	566.38	Joback Method
dvisc	0.0005551	Pa×s	502.04	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R30424&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume