2,2,2-Trichloroethyl nonadecanoate

Inchi: InChI=1S/C21H39Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20(25)26-19-21
InchiKey: HBCPZORCMRNRFJ-UHFFFAOYSA-N
Formula: C21H39Cl3O2
SMILES: CCCCCCCCCCCCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 429.89

Physical Properties

Property code	Value	Unit	Source
gf	-140.93	kJ/mol	Joback Method
hf	-777.54	kJ/mol	Joback Method
hfus	58.11	kJ/mol	Joback Method
hvap	83.36	kJ/mol	Joback Method
log10ws	-9.04		Crippen Method
logp	8.551		Crippen Method
mcvol	350.910	ml/mol	McGowan Method
pc	929.51	kPa	Joback Method
rinpol	2676.00		NIST Webbook
rinpol	2685.00		NIST Webbook
ripol	3089.00		NIST Webbook
ripol	3070.00		NIST Webbook
ripol	3084.00		NIST Webbook
ripol	3077.00		NIST Webbook
ripol	3084.00		NIST Webbook
tb	865.23	K	Joback Method
tc	1060.89	K	Joback Method
tf	490.77	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.47	J/mol×K	865.23	Joback Method
cpg	1148.42	J/mol×K	1028.28	Joback Method
cpg	1134.66	J/mol×K	995.67	Joback Method

cpg	1120.05	J/mol×K	963.06	Joback Method
cpg	1104.51	J/mol×K	930.45	Joback Method
cpg	1088.00	J/mol×K	897.84	Joback Method
cpg	1161.38	J/mol×K	1060.89	Joback Method
dvisc	0.0000314	Pa×s	865.23	Joback Method
dvisc	0.0000427	Pa×s	802.82	Joback Method
dvisc	0.0000610	Pa×s	740.41	Joback Method
dvisc	0.0000933	Pa×s	678.00	Joback Method
dvisc	0.0001553	Pa×s	615.59	Joback Method
dvisc	0.0002902	Pa×s	553.18	Joback Method
dvisc	0.0006356	Pa×s	490.77	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=R30474&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