2,2,2-Trichloroethyl heptadecanoate

Inchi: InChI=1S/C19H35Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-18(23)24-17-19(20,21
InchiKey: KIXAEYLIBITQBV-UHFFFAOYSA-N
Formula: C19H35Cl3O2
SMILES: CCCCCCCCCCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 401.84

Physical Properties

Property code	Value	Unit	Source
gf	-157.77	kJ/mol	Joback Method
hf	-736.26	kJ/mol	Joback Method
hfus	52.93	kJ/mol	Joback Method
hvap	78.90	kJ/mol	Joback Method
log10ws	-8.20		Crippen Method
logp	7.771		Crippen Method
mcvol	322.730	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	2474.00		NIST Webbook
rinpol	2481.00		NIST Webbook
rinpol	2481.00		NIST Webbook
ripol	2873.00		NIST Webbook
ripol	2873.00		NIST Webbook
ripol	2883.00		NIST Webbook
ripol	2867.00		NIST Webbook
ripol	2849.00		NIST Webbook
ripol	2873.00		NIST Webbook
ripol	2849.00		NIST Webbook
tb	819.47	K	Joback Method
tc	1009.85	K	Joback Method
tf	468.23	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	950.09	J/mol×K	819.47	Joback Method
cpg	966.83	J/mol×K	851.20	Joback Method
cpg	982.61	J/mol×K	882.93	Joback Method
cpg	997.49	J/mol×K	914.66	Joback Method
cpg	1011.50	J/mol×K	946.39	Joback Method
cpg	1024.70	J/mol×K	978.12	Joback Method
cpg	1037.14	J/mol×K	1009.85	Joback Method
dvisc	0.0008266	Pa×s	468.23	Joback Method
dvisc	0.0003848	Pa×s	526.77	Joback Method
dvisc	0.0002087	Pa×s	585.31	Joback Method
dvisc	0.0001265	Pa×s	643.85	Joback Method
dvisc	0.0000834	Pa×s	702.39	Joback Method
dvisc	0.0000586	Pa×s	760.93	Joback Method
dvisc	0.0000433	Pa×s	819.47	Joback Method

Sources

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=R30438&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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