Heptadecyl trichloroacetate

Inchi: InChI=1S/C19H35Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-24-18(23)19(20,21
InchiKey: VNNJRRWQDZVURW-UHFFFAOYSA-N
Formula: C19H35Cl3O2
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(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	2471.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R146226&Units=SI
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

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