

Trichloroacetic acid, tetradecyl ester

Other names:	Trichloroacetic acid, myristyl ester Tetradecyl trichloroacetate
Inchi:	InChI=1S/C16H29Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-21-15(20)16(17,18)19/h2-14
InchiKey:	CAUJGQDJKZXWDE-UHFFFAOYSA-N
Formula:	C16H29Cl3O2
SMILES:	CCCCCCCCCCCCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	359.76
CAS:	74339-52-9

Physical Properties

Property code	Value	Unit	Source
gf	-183.03	kJ/mol	Joback Method
hf	-674.34	kJ/mol	Joback Method
hfus	45.16	kJ/mol	Joback Method
hvap	72.22	kJ/mol	Joback Method
log10ws	-6.94		Crippen Method
logp	6.601		Crippen Method
mcvol	280.460	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	2163.50		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2163.50		NIST Webbook
rinpol	2171.00		NIST Webbook
rinpol	2174.00		NIST Webbook
ripol	2580.00		NIST Webbook
ripol	2580.00		NIST Webbook
tb	750.83	K	Joback Method
tc	938.56	K	Joback Method
tf	434.42	K	Joback Method
vc	1.091	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	776.02	J/molxK	750.83	Joback Method
cpg	791.67	J/molxK	782.12	Joback Method
cpg	806.45	J/molxK	813.41	Joback Method
cpg	820.39	J/molxK	844.69	Joback Method
cpg	833.54	J/molxK	875.98	Joback Method
cpg	845.93	J/molxK	907.27	Joback Method
cpg	857.60	J/molxK	938.56	Joback Method
dvisc	0.0011988	Paxs	434.42	Joback Method
dvisc	0.0005763	Paxs	487.16	Joback Method
dvisc	0.0003196	Paxs	539.89	Joback Method
dvisc	0.0001969	Paxs	592.62	Joback Method
dvisc	0.0001313	Paxs	645.36	Joback Method
dvisc	0.0000930	Paxs	698.10	Joback Method
dvisc	0.0000692	Paxs	750.83	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C74339529&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

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

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