Trichloroacetic acid, 2-naphthyl ester

Inchi: InChI=1S/C12H7Cl3O2/c13-12(14,15)11(16)17-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H
InchiKey: CXHQPDVKRPVPJV-UHFFFAOYSA-N
Formula: C12H7Cl3O2
SMILES: O=C(Oc1ccc2ccccc2c1)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 289.54

Physical Properties

Property code	Value	Unit	Source
gf	-7.28	kJ/mol	Joback Method
hf	-175.65	kJ/mol	Joback Method
hfus	25.47	kJ/mol	Joback Method
hvap	67.90	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.115		Crippen Method
mcvol	180.880	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1944.00		NIST Webbook
rinpol	1944.00		NIST Webbook
tb	709.95	K	Joback Method
tc	968.33	K	Joback Method
tf	460.98	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.12	J/mol×K	709.95	Joback Method
cpg	417.31	J/mol×K	753.01	Joback Method
cpg	426.48	J/mol×K	796.08	Joback Method
cpg	434.77	J/mol×K	839.14	Joback Method
cpg	442.29	J/mol×K	882.20	Joback Method
cpg	449.15	J/mol×K	925.27	Joback Method
cpg	455.48	J/mol×K	968.33	Joback Method
dvisc	0.0012227	Pa×s	460.98	Joback Method

dvisc	0.0008174	Pa×s	502.48	Joback Method
dvisc	0.0005811	Pa×s	543.97	Joback Method
dvisc	0.0004336	Pa×s	585.47	Joback Method
dvisc	0.0003363	Pa×s	626.96	Joback Method
dvisc	0.0002692	Pa×s	668.46	Joback Method
dvisc	0.0002212	Pa×s	709.95	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=U307724&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume