

1-Naphthoic acid, 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C13H9Cl3O2/c14-13(15,16)8-18-12(17)11-7-3-5-9-4-1-2-6-10(9)11/h1-7H,8H2
InchiKey:	SQDBIAIEUYOBDO-UHFFFAOYSA-N
Formula:	C13H9Cl3O2
SMILES:	O=C(OCC(Cl)(Cl)Cl)c1cccc2ccccc12
Mol. weight [g/mol]:	303.57

Physical Properties

Property code	Value	Unit	Source
gf	1.14	kJ/mol	Joback Method
hf	-196.29	kJ/mol	Joback Method
hfus	28.06	kJ/mol	Joback Method
hvap	70.12	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.367		Crippen Method
mvol	194.970	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	2192.00		NIST Webbook
rinpol	2192.00		NIST Webbook
tb	732.83	K	Joback Method
tc	985.33	K	Joback Method
tf	472.25	K	Joback Method
vc	0.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.84	J/molxK	732.83	Joback Method
cpg	467.67	J/molxK	774.91	Joback Method
cpg	477.50	J/molxK	817.00	Joback Method
cpg	486.44	J/molxK	859.08	Joback Method
cpg	494.62	J/molxK	901.16	Joback Method
cpg	502.14	J/molxK	943.24	Joback Method
cpg	509.13	J/molxK	985.33	Joback Method
dvisc	0.0011416	Paxs	472.25	Joback Method

dvisc	0.0007518	Paxs	515.68	Joback Method
dvisc	0.0005283	Paxs	559.11	Joback Method
dvisc	0.0003907	Paxs	602.54	Joback Method
dvisc	0.0003008	Paxs	645.97	Joback Method
dvisc	0.0002394	Paxs	689.40	Joback Method
dvisc	0.0001957	Paxs	732.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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