Dichloroacetic acid, 2-naphthyl ester

Inchi: InChI=1S/C12H8Cl2O2/c13-11(14)12(15)16-10-6-5-8-3-1-2-4-9(8)7-10/h1-7,11H
InchiKey: BINBEEOLDVVDPS-UHFFFAOYSA-N
Formula: C12H8Cl2O2
SMILES: O=C(Oc1ccc2ccccc2c1)C(Cl)Cl
Mol. weight [g/mol]: 255.10

Physical Properties

Property code	Value	Unit	Source
gf	-0.63	kJ/mol	Joback Method
hf	-156.44	kJ/mol	Joback Method
hfus	25.17	kJ/mol	Joback Method
hvap	64.42	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.549		Crippen Method
mcvol	168.640	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1859.00		NIST Webbook
tb	675.31	K	Joback Method
tc	921.67	K	Joback Method
tf	413.64	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.57	J/mol×K	675.31	Joback Method
cpg	394.91	J/mol×K	716.37	Joback Method
cpg	405.28	J/mol×K	757.43	Joback Method
cpg	414.77	J/mol×K	798.49	Joback Method
cpg	423.42	J/mol×K	839.55	Joback Method
cpg	431.33	J/mol×K	880.61	Joback Method
cpg	438.55	J/mol×K	921.67	Joback Method
dvisc	0.0015253	Pa×s	413.64	Joback Method
dvisc	0.0009902	Pa×s	457.25	Joback Method

dvisc	0.0006931	Pa×s	500.86	Joback Method
dvisc	0.0005136	Pa×s	544.48	Joback Method
dvisc	0.0003979	Pa×s	588.09	Joback Method
dvisc	0.0003194	Pa×s	631.70	Joback Method
dvisc	0.0002637	Pa×s	675.31	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307590&Units=SI

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