Chloroacetic acid, 2-naphthyl ester

Inchi: InChI=1S/C12H9ClO2/c13-8-12(14)15-11-6-5-9-3-1-2-4-10(9)7-11/h1-7H,8H2
InchiKey: DQHZHTWQJQJIKE-UHFFFAOYSA-N
Formula: C12H9ClO2
SMILES: O=C(CCl)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 220.65

Physical Properties

Property code	Value	Unit	Source
gf	13.74	kJ/mol	Joback Method
hf	-135.42	kJ/mol	Joback Method
hfus	24.49	kJ/mol	Joback Method
hvap	60.42	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.984		Crippen Method
mcvol	156.400	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	1799.00		NIST Webbook
tb	638.32	K	Joback Method
tc	876.81	K	Joback Method
tf	398.72	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.57	J/mol×K	638.32	Joback Method
cpg	372.75	J/mol×K	678.07	Joback Method
cpg	383.98	J/mol×K	717.82	Joback Method
cpg	394.34	J/mol×K	757.57	Joback Method
cpg	403.87	J/mol×K	797.31	Joback Method
cpg	412.63	J/mol×K	837.06	Joback Method
cpg	420.70	J/mol×K	876.81	Joback Method
dvisc	0.0014192	Pa×s	398.72	Joback Method
dvisc	0.0009705	Pa×s	438.65	Joback Method

dvisc	0.0007071	Pa×s	478.59	Joback Method
dvisc	0.0005409	Pa×s	518.52	Joback Method
dvisc	0.0004300	Pa×s	558.45	Joback Method
dvisc	0.0003524	Pa×s	598.39	Joback Method
dvisc	0.0002961	Pa×s	638.32	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307718&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