

1-Naphthaleneacetic acid, 2,2-dichloroethyl ester

Inchi:	InChI=1S/C14H12Cl2O2/c15-13(16)9-18-14(17)8-11-6-3-5-10-4-1-2-7-12(10)11/h1-7,13H
InchiKey:	IGHHBAOWILUFHE-UHFFFAOYSA-N
Formula:	C14H12Cl2O2
SMILES:	O=C(Cc1cccc2ccccc12)OCC(Cl)Cl
Mol. weight [g/mol]:	283.15

Physical Properties

Property code	Value	Unit	Source
gf	16.21	kJ/mol	Joback Method
hf	-197.72	kJ/mol	Joback Method
hfus	30.35	kJ/mol	Joback Method
hvap	68.87	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.729		Crippen Method
mvol	196.820	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	2467.00		NIST Webbook
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tb	721.07	K	Joback Method
tc	957.34	K	Joback Method
tf	436.18	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.68	J/molxK	721.07	Joback Method
cpg	496.23	J/molxK	760.45	Joback Method
cpg	507.79	J/molxK	799.83	Joback Method
cpg	518.43	J/molxK	839.21	Joback Method
cpg	528.22	J/molxK	878.58	Joback Method
cpg	537.25	J/molxK	917.96	Joback Method
cpg	545.56	J/molxK	957.34	Joback Method
dvisc	0.0013857	Paxs	436.18	Joback Method

dvisc	0.0008712	Paxs	483.66	Joback Method
dvisc	0.0005951	Paxs	531.14	Joback Method
dvisc	0.0004327	Paxs	578.62	Joback Method
dvisc	0.0003303	Paxs	626.11	Joback Method
dvisc	0.0002618	Paxs	673.59	Joback Method
dvisc	0.0002140	Paxs	721.07	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=U415046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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