Diallyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 1,2-di-2-propen-1-yl ester
	1,2-Benzenedicarboxylic acid, di-2-propenyl ester
	Allyl phthalate
	DAP monomer
	Dapon 35
	Dapon R
	Diallyl ester o-phthalic acid
	Diallyl ester of phthalic acid
	Diallylester kyseliny ftalove
	Diallylester phthalic acid
	NCI-C50657
	NSC 7667
	Phthalic acid, diallyl ester
	diprop-2-enyl benzene-1,2-dicarboxylate
	o-Phthalic acid, diallyl ester
Inchi:	InChI=1S/C14H14O4/c1-3-9-17-13(15)11-7-5-6-8-12(11)14(16)18-10-4-2/h3-8H,1-2,9-10
InchiKey:	QUDWYFHPNIMBFC-UHFFFAOYSA-N
Formula:	C14H14O4
SMILES:	C=CCOC(=O)c1ccccc1C(=O)OCC=C
Mol. weight [g/mol]:	246.26
CAS:	131-17-9

Physical Properties

Property code	Value	Unit	Source
chl	-6957.60 ± 7.10	kJ/mol	NIST Webbook
chl	-6960.10	kJ/mol	NIST Webbook
gf	-122.38	kJ/mol	Joback Method
hf	-345.97	kJ/mol	Joback Method
hfl	-549.80	kJ/mol	NIST Webbook
hfl	-552.40 ± 7.10	kJ/mol	NIST Webbook
hfus	28.68	kJ/mol	Joback Method
hvap	66.67	kJ/mol	Joback Method
log10ws	-3.34		Aqueous Solubility Prediction Method
logp	2.372		Crippen Method
mcvol	190.640	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method

rinpol	1698.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1718.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1692.00		NIST Webbook
tb	697.32	K	Joback Method
tc	910.28	K	Joback Method
tf	427.28	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.72	J/mol×K	697.32	Joback Method
cpg	550.00	J/mol×K	874.79	Joback Method
cpg	540.24	J/mol×K	839.30	Joback Method
cpg	529.64	J/mol×K	803.80	Joback Method
cpg	518.21	J/mol×K	768.31	Joback Method
cpg	505.90	J/mol×K	732.81	Joback Method
cpg	558.95	J/mol×K	910.28	Joback Method
dvisc	0.0001321	Pa×s	697.32	Joback Method
dvisc	0.0001645	Pa×s	652.31	Joback Method
dvisc	0.0002116	Pa×s	607.31	Joback Method
dvisc	0.0002834	Pa×s	562.30	Joback Method
dvisc	0.0003993	Pa×s	517.29	Joback Method
dvisc	0.0006008	Pa×s	472.29	Joback Method
dvisc	0.0009851	Pa×s	427.28	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	439.20	K	0.70	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C131179&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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