DIALLYL ISOPHTHALATE

Other names:	1,3-Benzenedicarboxylic acid, di-2-propenyl ester
	Di-2-Propenyl isophthalate
	Isophthalic acid, diallyl ester
	Dapon M
	Isophthalic acid, di-(2-propenyl) ester
Inchi:	InChI=1S/C14H14O4/c1-3-8-17-13(15)11-6-5-7-12(10-11)14(16)18-9-4-2/h3-7,10H,1-2,8
InchiKey:	OOORLLSLMPBSPT-UHFFFAOYSA-N
Formula:	C14H14O4
SMILES:	C=CCOC(=O)c1cccc(C(=O)OCC=C)c1
Mol. weight [g/mol]:	246.26

Physical Properties

Property code	Value	Unit	Source
af	0.6951		Cheméo Relay (1.0)
hf	-521.66	kJ/mol	Cheméo Relay (1.0)
hfus	28.68	kJ/mol	Joback Method
hvap	76.47	kJ/mol	Cheméo Relay (1.0)
ie	9.30	eV	Cheméo Relay (1.0)
log10ws	-3.62		Cheméo Relay (1.0)
logp	2.372		Crippen Method
mcvol	190.640	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
tb	606.71	K	Cheméo Relay (1.0)
tc	790.40	K	Cheméo Relay (1.0)
tf	296.61	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.72	J/mol×K	697.32	Joback Method
cpg	505.90	J/mol×K	732.81	Joback Method
cpg	518.21	J/mol×K	768.31	Joback Method
cpg	529.64	J/mol×K	803.80	Joback Method
cpg	540.24	J/mol×K	839.30	Joback Method

cpg	550.00	J/mol×K	874.79	Joback Method
cpg	558.95	J/mol×K	910.28	Joback Method
dvisc	0.0009851	Pa×s	427.28	Joback Method
dvisc	0.0006008	Pa×s	472.29	Joback Method
dvisc	0.0003993	Pa×s	517.29	Joback Method
dvisc	0.0002834	Pa×s	562.30	Joback Method
dvisc	0.0002116	Pa×s	607.31	Joback Method
dvisc	0.0001645	Pa×s	652.31	Joback Method
dvisc	0.0001321	Pa×s	697.32	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1087214&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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