

1,4-Benzenedicarboxylic acid, di-2-propenyl ester

Other names:	Diallyl terephthalate Terephthalic acid, diallyl ester Diallyl ester of terephthalic acid
Inchi:	InChI=1S/C14H14O4/c1-3-9-17-13(15)11-5-7-12(8-6-11)14(16)18-10-4-2/h3-8H,1-2,9-10
InchiKey:	ZDNFTNPFYCKVTB-UHFFFAOYSA-N
Formula:	C14H14O4
SMILES:	C=CCOC(=O)c1ccc(C(=O)OCC=C)cc1
Mol. weight [g/mol]:	246.26
CAS:	1026-92-2

Physical Properties

Property code	Value	Unit	Source
gf	-122.38	kJ/mol	Joback Method
hf	-345.97	kJ/mol	Joback Method
hfus	28.68	kJ/mol	Joback Method
hvap	66.67	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.372		Crippen Method
mcvol	190.640	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
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/molxK	697.32	Joback Method
cpg	550.00	J/molxK	874.79	Joback Method
cpg	540.24	J/molxK	839.30	Joback Method
cpg	529.64	J/molxK	803.80	Joback Method
cpg	518.21	J/molxK	768.31	Joback Method
cpg	505.90	J/molxK	732.81	Joback Method

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1026922&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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