Diprop-2-ynyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, diprop-2-ynyl ester
Diprop-2-ynyl-1,2-benzenedicarboxylate
Inchi: InChI=1S/C14H10O4/c1-3-9-17-13(15)11-7-5-6-8-12(11)14(16)18-10-4-2/h1-2,5-8H,9-10
InchiKey: NQXDCRARZBUWHX-UHFFFAOYSA-N
Formula: C14H10O4
SMILES: C#CCOC(=O)c1ccccc1C(=O)OCC#C
Mol. weight [g/mol]: 242.23

Physical Properties

Property code	Value	Unit	Source
gf	148.08	kJ/mol	Joback Method
hf	-13.03	kJ/mol	Joback Method
hfus	37.19	kJ/mol	Joback Method
hvap	67.72	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	1.267		Crippen Method
mcvol	182.040	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1793.00		NIST Webbook
rinpol	1793.00		NIST Webbook
tb	684.20	K	Joback Method
tc	915.99	K	Joback Method
tf	524.74	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.92	J/mol×K	684.20	Joback Method
cpg	457.92	J/mol×K	722.83	Joback Method
cpg	469.05	J/mol×K	761.46	Joback Method
cpg	479.32	J/mol×K	800.09	Joback Method
cpg	488.76	J/mol×K	838.73	Joback Method
cpg	497.40	J/mol×K	877.36	Joback Method

cpg	505.24	J/mol×K	915.99	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=U373493&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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