(E)-2-((Hex-3-enyloxy)carbonyl)benzoic acid

Other names: Phthalic acid, mono-(E)-hex-3-enyl ester
(E)-Hex-3-enyl hydrogen phthalate
Mono-(E)-hex-3-enyl phthalate
Inchi: InChI=1S/C14H16O4/c1-2-3-4-7-10-18-14(17)12-9-6-5-8-11(12)13(15)16/h3-6,8-9H,2,7,1
InchiKey: UOYDHCVOIGSHCY-ONEGZZNKSA-N
Formula: C14H16O4
SMILES: CCC=CCCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 248.27

Physical Properties

Property code	Value	Unit	Source
gf	-249.66	kJ/mol	Joback Method
hf	-499.62	kJ/mol	Joback Method
hfus	34.34	kJ/mol	Joback Method
hvap	82.23	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.898		Crippen Method
mcvol	194.940	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	2015.00		NIST Webbook
tb	777.88	K	Joback Method
tc	982.21	K	Joback Method
tf	464.31	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.05	J/mol×K	777.88	Joback Method
cpg	554.44	J/mol×K	811.94	Joback Method
cpg	565.08	J/mol×K	845.99	Joback Method
cpg	575.00	J/mol×K	880.05	Joback Method
cpg	584.23	J/mol×K	914.10	Joback Method
cpg	592.80	J/mol×K	948.16	Joback Method

cpg	600.75	J/mol×K	982.21	Joback Method
dvisc	0.0007698	Pa×s	464.31	Joback Method
dvisc	0.0003276	Pa×s	516.57	Joback Method
dvisc	0.0001631	Pa×s	568.83	Joback Method
dvisc	0.0000913	Pa×s	621.10	Joback Method
dvisc	0.0000559	Pa×s	673.36	Joback Method
dvisc	0.0000368	Pa×s	725.62	Joback Method
dvisc	0.0000256	Pa×s	777.88	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=U373679&Units=SI

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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