

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

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,2,7,14H
InchiKey:	UOYDHCVOIGSHCY-ARJAWSKDSA-N
Formula:	C14H16O4
SMILES:	CCC=CCCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]:	248.27
CAS:	298712-38-6

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	2019.00		NIST Webbook
rinpol	2019.00		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/molxK	777.88	Joback Method
cpg	554.44	J/molxK	811.94	Joback Method
cpg	565.08	J/molxK	845.99	Joback Method
cpg	575.00	J/molxK	880.05	Joback Method
cpg	584.23	J/molxK	914.10	Joback Method
cpg	592.80	J/molxK	948.16	Joback Method
cpg	600.75	J/molxK	982.21	Joback Method

dvisc	0.0007698	Paxs	464.31	Joback Method
dvisc	0.0003276	Paxs	516.57	Joback Method
dvisc	0.0001631	Paxs	568.83	Joback Method
dvisc	0.0000913	Paxs	621.10	Joback Method
dvisc	0.0000559	Paxs	673.36	Joback Method
dvisc	0.0000368	Paxs	725.62	Joback Method
dvisc	0.0000256	Paxs	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=C298712386&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
mvol:	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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