Phenylacetic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C16H22O2/c1-3-4-5-7-10-14(2)18-16(17)13-15-11-8-6-9-12-15/h6-12,14H,3-5,
InchiKey: SHXMLJPUXCFKKS-JXMROGBWSA-N
Formula: C16H22O2
SMILES: CCCCC=CC(C)OC(=O)Cc1ccccc1
Mol. weight [g/mol]: 246.34

Physical Properties

Property code	Value	Unit	Source
gf	40.11	kJ/mol	Joback Method
hf	-269.90	kJ/mol	Joback Method
hfus	30.70	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.907		Crippen Method
mcvol	215.680	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	1738.10		NIST Webbook
tb	672.17	K	Joback Method
tc	878.02	K	Joback Method
tf	348.58	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.50	J/mol×K	672.17	Joback Method
cpg	653.76	J/mol×K	843.71	Joback Method
cpg	640.58	J/mol×K	809.41	Joback Method
cpg	626.51	J/mol×K	775.10	Joback Method
cpg	611.51	J/mol×K	740.79	Joback Method
cpg	595.52	J/mol×K	706.48	Joback Method
cpg	666.08	J/mol×K	878.02	Joback Method
dvisc	0.0000972	Pa×s	672.17	Joback Method
dvisc	0.0001299	Pa×s	618.24	Joback Method

dvisc	0.0001834	Pa×s	564.31	Joback Method
dvisc	0.0002787	Pa×s	510.38	Joback Method
dvisc	0.0004673	Pa×s	456.44	Joback Method
dvisc	0.0008999	Pa×s	402.51	Joback Method
dvisc	0.0021230	Pa×s	348.58	Joback Method

Sources

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=U292533&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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