

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

Inchi:	InChI=1S/C17H24O2/c1-3-4-5-7-10-15(2)19-17(18)14-13-16-11-8-6-9-12-16/h6-12,15H,3
InchiKey:	MAKKQAYXFZLERU-JXMROGBWSA-N
Formula:	C17H24O2
SMILES:	CCCCC=CC(C)OC(=O)CCc1ccccc1
Mol. weight [g/mol]:	260.37

Physical Properties

Property code	Value	Unit	Source
gf	48.53	kJ/mol	Joback Method
hf	-290.54	kJ/mol	Joback Method
hfus	33.29	kJ/mol	Joback Method
hvap	64.44	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.297		Crippen Method
mvol	229.770	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	1829.00		NIST Webbook
rinpol	1829.00		NIST Webbook
tb	695.05	K	Joback Method
tc	898.29	K	Joback Method
tf	359.85	K	Joback Method
vc	0.877	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.80	J/molxK	695.05	Joback Method
cpg	709.54	J/molxK	864.41	Joback Method
cpg	696.09	J/molxK	830.54	Joback Method
cpg	681.73	J/molxK	796.67	Joback Method
cpg	666.43	J/molxK	762.80	Joback Method
cpg	650.13	J/molxK	728.92	Joback Method
cpg	722.14	J/molxK	898.29	Joback Method
dvisc	0.0000864	Paxs	695.05	Joback Method

dvisc	0.0001158	Paxs	639.18	Joback Method
dvisc	0.0001641	Paxs	583.32	Joback Method
dvisc	0.0002505	Paxs	527.45	Joback Method
dvisc	0.0004224	Paxs	471.58	Joback Method
dvisc	0.0008198	Paxs	415.72	Joback Method
dvisc	0.0019547	Paxs	359.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299175&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
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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