3-Phenylpropionic acid, undec-2-enyl ester

Inchi: InChI=1S/C20H30O2/c1-2-3-4-5-6-7-8-9-13-18-22-20(21)17-16-19-14-11-10-12-15-19/h9
InchiKey: PPSMSYBRCIUADP-UKTHLTGXSA-N
Formula: C20H30O2
SMILES: CCCCCCCCC=CCOC(=O)CCc1ccccc1
Mol. weight [g/mol]: 302.45

Physical Properties

Property code	Value	Unit	Source
gf	76.23	kJ/mol	Joback Method
hf	-347.18	kJ/mol	Joback Method
hfus	44.59	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.469		Crippen Method
mcvol	272.040	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook
tb	764.13	K	Joback Method
tc	959.70	K	Joback Method
tf	408.66	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.99	J/mol×K	764.13	Joback Method
cpg	881.24	J/mol×K	927.11	Joback Method
cpg	867.26	J/mol×K	894.51	Joback Method
cpg	852.39	J/mol×K	861.92	Joback Method
cpg	836.59	J/mol×K	829.32	Joback Method
cpg	819.80	J/mol×K	796.73	Joback Method
cpg	894.39	J/mol×K	959.70	Joback Method
dvisc	0.0000643	Pa×s	764.13	Joback Method

dvisc	0.0000853	Pa×s	704.88	Joback Method
dvisc	0.0001193	Pa×s	645.64	Joback Method
dvisc	0.0001784	Pa×s	586.39	Joback Method
dvisc	0.0002920	Pa×s	527.15	Joback Method
dvisc	0.0005415	Pa×s	467.90	Joback Method
dvisc	0.0012013	Pa×s	408.66	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=U299179&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