

Phenylacetic acid, undec-2-enyl ester

Inchi:	InChI=1S/C19H28O2/c1-2-3-4-5-6-7-8-9-13-16-21-19(20)17-18-14-11-10-12-15-18/h9-15
InchiKey:	FWVZPQUCMWVYEI-UKTHLTGXSA-N
Formula:	C19H28O2
SMILES:	CCCCCCCCC=CCOC(=O)Cc1ccccc1
Mol. weight [g/mol]:	288.42

Physical Properties

Property code	Value	Unit	Source
gf	67.81	kJ/mol	Joback Method
hf	-326.54	kJ/mol	Joback Method
hfus	42.00	kJ/mol	Joback Method
hvap	69.28	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.079		Crippen Method
mcvol	257.950	ml/mol	McGowan Method
pc	1464.61	kPa	Joback Method
rinpola	2150.30		NIST Webbook
tb	741.25	K	Joback Method
tc	937.78	K	Joback Method
tf	397.39	K	Joback Method
vc	0.996	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.37	J/molxK	741.25	Joback Method
cpg	822.53	J/molxK	905.02	Joback Method
cpg	808.75	J/molxK	872.27	Joback Method
cpg	794.09	J/molxK	839.51	Joback Method
cpg	778.50	J/molxK	806.76	Joback Method
cpg	761.95	J/molxK	774.00	Joback Method
cpg	835.48	J/molxK	937.78	Joback Method
dvisc	0.0000731	Paxs	741.25	Joback Method
dvisc	0.0000968	Paxs	683.94	Joback Method

dvisc	0.0001348	Paxs	626.63	Joback Method
dvisc	0.0002006	Paxs	569.32	Joback Method
dvisc	0.0003265	Paxs	512.01	Joback Method
dvisc	0.0006009	Paxs	454.70	Joback Method
dvisc	0.0013184	Paxs	397.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292537&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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