2-PHENETHYL-beta-PHENYLPROPIONATE

Other names: 3-Phenylpropionic acid, 2-phenylethyl ester
2-Phenylethyl 3-phenylpropanoate
Inchi: InChI=1S/C17H18O2/c18-17(12-11-15-7-3-1-4-8-15)19-14-13-16-9-5-2-6-10-16/h1-10H,1
InchiKey: QQNDZUIFXZRWFO-UHFFFAOYSA-N
Formula: C17H18O2
SMILES: O=C(CCc1ccccc1)OCCc1ccccc1
Mol. weight [g/mol]: 254.33

Physical Properties

Property code	Value	Unit	Source
hf	-208.11	kJ/mol	Cheméo Relay (1.0)
hfus	30.66	kJ/mol	Joback Method
hvap	97.14	kJ/mol	Cheméo Relay (1.0)
ie	8.52	eV	Cheméo Relay (1.0)
log10ws	-4.06		Cheméo Relay (1.0)
logp	3.405		Crippen Method
mcvol	210.310	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	2049.30		NIST Webbook
rinpol	2015.00		NIST Webbook
ripol	2747.00		NIST Webbook
ripol	2825.00		NIST Webbook
ripol	2747.00		NIST Webbook
tb	621.56	K	Cheméo Relay (1.0)
tf	274.81	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.19	J/mol×K	718.01	Joback Method
cpg	588.63	J/mol×K	756.11	Joback Method
cpg	603.83	J/mol×K	794.22	Joback Method
cpg	617.83	J/mol×K	832.32	Joback Method
cpg	630.71	J/mol×K	870.43	Joback Method

cpg	642.51	J/mol×K	908.53	Joback Method
cpg	653.31	J/mol×K	946.64	Joback Method
dvisc	0.0013370	Pa×s	406.35	Joback Method
dvisc	0.0006949	Pa×s	458.29	Joback Method
dvisc	0.0004126	Pa×s	510.24	Joback Method
dvisc	0.0002698	Pa×s	562.18	Joback Method
dvisc	0.0001896	Pa×s	614.12	Joback Method
dvisc	0.0001407	Pa×s	666.07	Joback Method
dvisc	0.0001091	Pa×s	718.01	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28049107&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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