PROPANOIC ACID, 2-PHENOXY-, METHYL ESTER

Other names: Methyl 2-phenoxypropionate
Inchi: InChI=1S/C10H12O3/c1-8(10(11)12-2)13-9-6-4-3-5-7-9/h3-8H,1-2H3
InchiKey: KIBRBMKSBVQDMK-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: COC(=O)C(C)Oc1ccccc1
Mol. weight [g/mol]: 180.20

Physical Properties

Property code	Value	Unit	Source
af	0.4918		Cheméo Relay (1.0)
hf	-445.05	kJ/mol	Cheméo Relay (1.0)
hfus	16.15	kJ/mol	Joback Method
hvap	66.57	kJ/mol	Cheméo Relay (1.0)
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-1.70		Cheméo Relay (1.0)
logp	1.627		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
tb	498.91	K	Cheméo Relay (1.0)
tc	701.06	K	Cheméo Relay (1.0)
tf	297.71	K	Cheméo Relay (1.0)
vc	0.517	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.75	J/mol×K	553.15	Joback Method
cpg	338.43	J/mol×K	588.99	Joback Method
cpg	351.37	J/mol×K	624.82	Joback Method
cpg	363.58	J/mol×K	660.66	Joback Method
cpg	375.04	J/mol×K	696.50	Joback Method
cpg	385.78	J/mol×K	732.34	Joback Method
cpg	395.79	J/mol×K	768.17	Joback Method
dvisc	0.0022528	Pa×s	308.27	Joback Method

dvisc	0.0011324	Pa×s	349.08	Joback Method
dvisc	0.0006573	Pa×s	389.90	Joback Method
dvisc	0.0004230	Pa×s	430.71	Joback Method
dvisc	0.0002938	Pa×s	471.52	Joback Method
dvisc	0.0002163	Pa×s	512.34	Joback Method
dvisc	0.0001666	Pa×s	553.15	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2065249&Units=SI

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):

Legend

af: Acentric Factor
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.