11-PHENOXYUNDECANOIC ACID

Other names: 11-Phenoxyundecanoic acid
Inchi: InChI=1S/C17H26O3/c18-17(19)14-10-5-3-1-2-4-6-11-15-20-16-12-8-7-9-13-16/h7-9,12-
InchiKey: FRSQLPPSRJNREN-UHFFFAOYSA-N
Formula: C17H26O3
SMILES: O=C(O)CCCCCCCCCCOc1ccccc1
Mol. weight [g/mol]: 278.39

Physical Properties

Property code	Value	Unit	Source
af	1.0318		Cheméo Relay (1.0)
hf	-624.41	kJ/mol	Cheméo Relay (1.0)
hfus	40.70	kJ/mol	Joback Method
hvap	125.65	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-4.80		Cheméo Relay (1.0)
logp	4.661		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
tb	634.42	K	Cheméo Relay (1.0)
tc	848.71	K	Cheméo Relay (1.0)
tf	367.27	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.27	J/mol×K	783.51	Joback Method
cpg	734.92	J/mol×K	815.17	Joback Method
cpg	748.70	J/mol×K	846.83	Joback Method
cpg	761.64	J/mol×K	878.49	Joback Method
cpg	773.77	J/mol×K	910.15	Joback Method
cpg	785.12	J/mol×K	941.81	Joback Method
cpg	795.71	J/mol×K	973.47	Joback Method
dvisc	0.0011083	Pa×s	440.75	Joback Method
dvisc	0.0003879	Pa×s	497.88	Joback Method

dvisc	0.0001685	Pa×s	555.00	Joback Method
dvisc	0.0000856	Pa×s	612.13	Joback Method
dvisc	0.0000488	Pa×s	669.26	Joback Method
dvisc	0.0000304	Pa×s	726.38	Joback Method
dvisc	0.0000203	Pa×s	783.51	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	492.70	K	0.40	NIST Webbook

Sources

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=C7170447&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point