

Ethanol, 2-phenoxy-, propanoate

Other names:	Ethanol, 2-phenoxy-, propionate 2-Phenoxyethyl propionate Ethyleneglycol monophenyl ether propionate Propionic acid, 2-phenoxyethyl ester 2-Phenoxyethanol propionate Phenyloxyethyl propionate
Inchi:	InChI=1S/C11H14O3/c1-2-11(12)14-9-8-13-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3
InchiKey:	FKTSMIXZGPUSJB-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]:	194.23
CAS:	23495-12-7

Physical Properties

Property code	Value	Unit	Source
gf	-184.77	kJ/mol	Joback Method
hf	-410.86	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	53.92	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.019		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1436.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1447.00		NIST Webbook
ripol	2126.00		NIST Webbook
ripol	2126.00		NIST Webbook
tb	576.47	K	Joback Method
tc	783.57	K	Joback Method
tf	334.54	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.22	J/molxK	576.47	Joback Method
cpg	385.38	J/molxK	610.99	Joback Method
cpg	398.78	J/molxK	645.50	Joback Method
cpg	411.43	J/molxK	680.02	Joback Method
cpg	423.35	J/molxK	714.54	Joback Method
cpg	434.52	J/molxK	749.05	Joback Method
cpg	444.97	J/molxK	783.57	Joback Method
dvisc	0.0016964	Paxs	334.54	Joback Method
dvisc	0.0009299	Paxs	374.86	Joback Method
dvisc	0.0005728	Paxs	415.18	Joback Method
dvisc	0.0003845	Paxs	455.50	Joback Method
dvisc	0.0002753	Paxs	495.83	Joback Method
dvisc	0.0002073	Paxs	536.15	Joback Method
dvisc	0.0001625	Paxs	576.47	Joback Method

Sources

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=C23495127&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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