3-Phenoxypropyl acetate

Inchi: InChI=1S/C11H14O3/c1-10(12)13-8-5-9-14-11-6-3-2-4-7-11/h2-4,6-7H,5,8-9H2,1H3
InchiKey: FZOXUFODEISZLN-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CC(=O)OCCCOc1ccccc1
Mol. weight [g/mol]: 194.23

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	1502.00		NIST Webbook
rinpol	1502.00		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/mol×K	576.47	Joback Method
cpg	385.38	J/mol×K	610.99	Joback Method
cpg	398.78	J/mol×K	645.50	Joback Method
cpg	411.43	J/mol×K	680.02	Joback Method
cpg	423.35	J/mol×K	714.54	Joback Method
cpg	434.52	J/mol×K	749.05	Joback Method
cpg	444.97	J/mol×K	783.57	Joback Method
dvisc	0.0016964	Pa×s	334.54	Joback Method

dvisc	0.0009299	Pa×s	374.86	Joback Method
dvisc	0.0005728	Pa×s	415.18	Joback Method
dvisc	0.0003845	Pa×s	455.50	Joback Method
dvisc	0.0002753	Pa×s	495.83	Joback Method
dvisc	0.0002073	Pa×s	536.15	Joback Method
dvisc	0.0001625	Pa×s	576.47	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U378335&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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