Butyl 2-phenoxypropionate

Inchi: InChI=1S/C13H18O3/c1-3-4-10-15-13(14)11(2)16-12-8-6-5-7-9-12/h5-9,11H,3-4,10H2,1-
InchiKey: BNDNRTDZPSIZIY-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: CCCCOC(=O)C(C)Oc1ccccc1
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
gf	-170.37	kJ/mol	Joback Method
hf	-457.42	kJ/mol	Joback Method
hfus	23.92	kJ/mol	Joback Method
hvap	57.99	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.797		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	1492.00		NIST Webbook
tb	621.79	K	Joback Method
tc	826.70	K	Joback Method
tf	342.08	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.27	J/mol×K	621.79	Joback Method
cpg	540.60	J/mol×K	792.55	Joback Method
cpg	528.25	J/mol×K	758.39	Joback Method
cpg	515.06	J/mol×K	724.24	Joback Method
cpg	501.01	J/mol×K	690.09	Joback Method
cpg	486.08	J/mol×K	655.94	Joback Method
cpg	552.10	J/mol×K	826.70	Joback Method
dvisc	0.0001240	Pa×s	621.79	Joback Method
dvisc	0.0001630	Pa×s	575.17	Joback Method

dvisc	0.0002248	Pa×s	528.55	Joback Method
dvisc	0.0003299	Pa×s	481.94	Joback Method
dvisc	0.0005257	Pa×s	435.32	Joback Method
dvisc	0.0009365	Pa×s	388.70	Joback Method
dvisc	0.0019529	Pa×s	342.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541270&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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