

Butyl 2-phenoxybutyrate

Inchi:	InChI=1S/C14H20O3/c1-3-5-11-16-14(15)13(4-2)17-12-9-7-6-8-10-12/h6-10,13H,3-5,11H
InchiKey:	LANPZDBBZPZMQZ-UHFFFAOYSA-N
Formula:	C14H20O3
SMILES:	CCCCOC(=O)C(CC)Oc1ccccc1
Mol. weight [g/mol]:	236.31

Physical Properties

Property code	Value	Unit	Source
gf	-161.95	kJ/mol	Joback Method
hf	-478.06	kJ/mol	Joback Method
hfus	26.51	kJ/mol	Joback Method
hvap	60.21	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.187		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinsol	1565.00		NIST Webbook
tb	644.67	K	Joback Method
tc	846.70	K	Joback Method
tf	353.35	K	Joback Method
vc	0.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.88	J/molxK	644.67	Joback Method
cpg	594.36	J/molxK	813.03	Joback Method
cpg	581.65	J/molxK	779.36	Joback Method
cpg	568.06	J/molxK	745.68	Joback Method
cpg	553.58	J/molxK	712.01	Joback Method
cpg	538.19	J/molxK	678.34	Joback Method
cpg	606.21	J/molxK	846.70	Joback Method
dvisc	0.0001110	Paxs	644.67	Joback Method
dvisc	0.0001463	Paxs	596.12	Joback Method

dvisc	0.0002027	Paxs	547.56	Joback Method
dvisc	0.0002991	Paxs	499.01	Joback Method
dvisc	0.0004801	Paxs	450.46	Joback Method
dvisc	0.0008639	Paxs	401.90	Joback Method
dvisc	0.0018268	Paxs	353.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541265&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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