

Hexyl 2-phenoxybutyrate

Inchi:	InChI=1S/C16H24O3/c1-3-5-6-10-13-18-16(17)15(4-2)19-14-11-8-7-9-12-14/h7-9,11-12,
InchiKey:	MPOWEJRLFLCFNF-UHFFFAOYSA-N
Formula:	C16H24O3
SMILES:	CCCCCCOC(=O)C(CC)Oc1ccccc1
Mol. weight [g/mol]:	264.36

Physical Properties

Property code	Value	Unit	Source
gf	-145.11	kJ/mol	Joback Method
hf	-519.34	kJ/mol	Joback Method
hfus	31.69	kJ/mol	Joback Method
hvap	64.66	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.967		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinsol	1756.00		NIST Webbook
tb	690.43	K	Joback Method
tc	887.72	K	Joback Method
tf	375.89	K	Joback Method
vc	0.860	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.15	J/molxK	690.43	Joback Method
cpg	646.23	J/molxK	723.31	Joback Method
cpg	662.33	J/molxK	756.19	Joback Method
cpg	677.46	J/molxK	789.07	Joback Method
cpg	691.65	J/molxK	821.95	Joback Method
cpg	704.91	J/molxK	854.83	Joback Method
cpg	717.26	J/molxK	887.72	Joback Method
dvisc	0.0015621	Paxs	375.89	Joback Method
dvisc	0.0007200	Paxs	428.31	Joback Method

dvisc	0.0003930	Paxs	480.74	Joback Method
dvisc	0.0002416	Paxs	533.16	Joback Method
dvisc	0.0001620	Paxs	585.58	Joback Method
dvisc	0.0001161	Paxs	638.01	Joback Method
dvisc	0.0000874	Paxs	690.43	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=R543201&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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