

2-Methoxyethyl 2-phenoxypropionate

Inchi:	InChI=1S/C12H16O4/c1-10(12(13)15-9-8-14-2)16-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H
InchiKey:	BOTPINPRRBDDNR-UHFFFAOYSA-N
Formula:	C12H16O4
SMILES:	COCCOC(=O)C(C)Oc1ccccc1
Mol. weight [g/mol]:	224.25

Physical Properties

Property code	Value	Unit	Source
gf	-283.79	kJ/mol	Joback Method
hf	-569.00	kJ/mol	Joback Method
hfus	22.52	kJ/mol	Joback Method
hvap	58.17	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.643		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinsol	1512.00		NIST Webbook
tb	621.33	K	Joback Method
tc	827.26	K	Joback Method
tf	353.04	K	Joback Method
vc	0.653	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.02	J/molxK	621.33	Joback Method
cpg	460.94	J/molxK	655.65	Joback Method
cpg	475.05	J/molxK	689.97	Joback Method
cpg	488.33	J/molxK	724.30	Joback Method
cpg	500.80	J/molxK	758.62	Joback Method
cpg	512.44	J/molxK	792.94	Joback Method
cpg	523.26	J/molxK	827.26	Joback Method
dvisc	0.0014623	Paxs	353.04	Joback Method
dvisc	0.0007435	Paxs	397.75	Joback Method

dvisc	0.0004334	Paxs	442.47	Joback Method
dvisc	0.0002790	Paxs	487.19	Joback Method
dvisc	0.0001934	Paxs	531.90	Joback Method
dvisc	0.0001419	Paxs	576.62	Joback Method
dvisc	0.0001088	Paxs	621.33	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=R540599&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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