

2-Methoxyethyl 2-phenoxybutyrate

Inchi:	InChI=1S/C13H18O4/c1-3-12(13(14)16-10-9-15-2)17-11-7-5-4-6-8-11/h4-8,12H,3,9-10H
InchiKey:	PPSVYOYUSOJGIC-UHFFFAOYSA-N
Formula:	C13H18O4
SMILES:	CCC(Oc1ccccc1)C(=O)OCCOC
Mol. weight [g/mol]:	238.28

Physical Properties

Property code	Value	Unit	Source
gf	-275.37	kJ/mol	Joback Method
hf	-589.64	kJ/mol	Joback Method
hfus	25.11	kJ/mol	Joback Method
hvap	60.40	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.034		Crippen Method
mvol	189.450	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	1585.00		NIST Webbook
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tb	644.21	K	Joback Method
tc	847.20	K	Joback Method
tf	364.31	K	Joback Method
vc	0.710	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.95	J/molxK	644.21	Joback Method
cpg	565.75	J/molxK	813.37	Joback Method
cpg	553.72	J/molxK	779.54	Joback Method
cpg	540.82	J/molxK	745.70	Joback Method
cpg	527.06	J/molxK	711.87	Joback Method
cpg	512.44	J/molxK	678.04	Joback Method
cpg	576.92	J/molxK	847.20	Joback Method
dvisc	0.0000972	Paxs	644.21	Joback Method

dvisc	0.0001271	Paxs	597.56	Joback Method
dvisc	0.0001741	Paxs	550.91	Joback Method
dvisc	0.0002526	Paxs	504.26	Joback Method
dvisc	0.0003956	Paxs	457.61	Joback Method
dvisc	0.0006858	Paxs	410.96	Joback Method
dvisc	0.0013689	Paxs	364.31	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540584&Units=SI

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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