

3-Phenylpropionic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C15H22O3/c1-13(10-11-17-2)12-18-15(16)9-8-14-6-4-3-5-7-14/h3-7,13H,8-12H
InchiKey: WPOYFKUIUGDUNE-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: COCCC(C)COC(=O)CCc1ccccc1
Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
gf	-153.53	kJ/mol	Joback Method
hf	-498.70	kJ/mol	Joback Method
hfus	29.10	kJ/mol	Joback Method
hvap	62.44	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.835		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	1871.00		NIST Webbook
tb	667.55	K	Joback Method
tc	867.02	K	Joback Method
tf	364.62	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.87	J/mol×K	667.55	Joback Method
cpg	591.60	J/mol×K	700.80	Joback Method
cpg	607.37	J/mol×K	734.04	Joback Method
cpg	622.21	J/mol×K	767.29	Joback Method
cpg	636.13	J/mol×K	800.53	Joback Method
cpg	649.15	J/mol×K	833.78	Joback Method
cpg	661.27	J/mol×K	867.02	Joback Method
dvisc	0.0016953	Pa×s	364.62	Joback Method
dvisc	0.0007912	Pa×s	415.11	Joback Method

dvisc	0.0004356	Pa×s	465.60	Joback Method
dvisc	0.0002696	Pa×s	516.09	Joback Method
dvisc	0.0001817	Pa×s	566.57	Joback Method
dvisc	0.0001306	Pa×s	617.06	Joback Method
dvisc	0.0000987	Pa×s	667.55	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=U354740&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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