(3-methoxy-4-cyclohexylmethoxy-phenyl)-acetic acid, methyl ester

Inchi: InChI=1S/C17H24O4/c1-19-16-10-14(11-17(18)20-2)8-9-15(16)21-12-13-6-4-3-5-7-13/h8
InchiKey: GPRKKTJEDIYRNB-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: COC(=O)Cc1ccc(OCC2CCCCC2)c(OC)c1
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-234.06	kJ/mol	Joback Method
hf	-635.54	kJ/mol	Joback Method
hfus	30.05	kJ/mol	Joback Method
hvap	71.44	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.370		Crippen Method
mcvol	234.950	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	2165.90		NIST Webbook
rinpol	2165.90		NIST Webbook
tb	765.68	K	Joback Method
tc	984.87	K	Joback Method
tf	456.81	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.37	J/mol×K	765.68	Joback Method
cpg	725.78	J/mol×K	802.21	Joback Method
cpg	742.80	J/mol×K	838.74	Joback Method
cpg	758.43	J/mol×K	875.27	Joback Method
cpg	772.68	J/mol×K	911.81	Joback Method
cpg	785.54	J/mol×K	948.34	Joback Method
cpg	797.01	J/mol×K	984.87	Joback Method
dvisc	0.0006544	Pa×s	456.81	Joback Method

dvisc	0.0003695	Pa×s	508.29	Joback Method
dvisc	0.0002317	Pa×s	559.77	Joback Method
dvisc	0.0001572	Pa×s	611.25	Joback Method
dvisc	0.0001133	Pa×s	662.72	Joback Method
dvisc	0.0000856	Pa×s	714.20	Joback Method
dvisc	0.0000671	Pa×s	765.68	Joback Method

Sources

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=R158031&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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