

3-(3-methoxy-4-isopropoxy-phenyl)-2-methyl-propionic acid, methyl ester

Inchi: CC(C)C(=O)OCc1ccc(OC(C)C)c(OC)c1
InchiKey: ZWVUNIMYLWNFOX-UHFFFAOYSA-N

Formula: C15H22O4

SMILES: COC(=O)C(C)Cc1ccc(OC(C)C)c(OC)c1

Mol. weight [g/mol]: 266.33

Physical Properties

Property code	Value	Unit	Source
gf	-280.23	kJ/mol	Joback Method
hf	-659.14	kJ/mol	Joback Method
hfus	25.99	kJ/mol	Joback Method
hvap	65.78	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.834		Crippen Method
mcvol	217.630	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	1710.50		NIST Webbook
tb	699.49	K	Joback Method
tc	902.54	K	Joback Method
tf	396.89	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.47	J/molxK	699.49	Joback Method
cpg	618.85	J/molxK	733.33	Joback Method
cpg	634.28	J/molxK	767.17	Joback Method
cpg	648.75	J/molxK	801.01	Joback Method
cpg	662.26	J/molxK	834.85	Joback Method
cpg	674.81	J/molxK	868.70	Joback Method
cpg	686.38	J/molxK	902.54	Joback Method
dvisc	0.0008985	Paxs	396.89	Joback Method
dvisc	0.0004620	Paxs	447.32	Joback Method

dvisc	0.0002718	Paxs	497.76	Joback Method
dvisc	0.0001763	Paxs	548.19	Joback Method
dvisc	0.0001230	Paxs	598.62	Joback Method
dvisc	0.0000908	Paxs	649.06	Joback Method
dvisc	0.0000700	Paxs	699.49	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=R157909&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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