

(4-Isobutoxy-phenyl)-acetic acid, methyl ester

Inchi:	InChI=1S/C13H18O3/c1-10(2)9-16-12-6-4-11(5-7-12)8-13(14)15-3/h4-7,10H,8-9H2,1-3H
InchiKey:	KCTOGAHDQAKXEN-UHFFFAOYSA-N
Formula:	C13H18O3
SMILES:	COC(=O)Cc1ccc(OCC(C)C)cc1
Mol. weight [g/mol]:	222.28

Physical Properties

Property code	Value	Unit	Source
gf	-180.00	kJ/mol	Joback Method
hf	-468.89	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	58.65	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.437		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1606.10		NIST Webbook
rinpol	1606.10		NIST Webbook
tb	626.77	K	Joback Method
tc	832.59	K	Joback Method
tf	354.60	K	Joback Method
vc	0.692	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.86	J/molxK	626.77	Joback Method
cpg	539.46	J/molxK	798.29	Joback Method
cpg	527.21	J/molxK	763.98	Joback Method
cpg	514.14	J/molxK	729.68	Joback Method
cpg	500.22	J/molxK	695.38	Joback Method
cpg	485.46	J/molxK	661.07	Joback Method
cpg	550.88	J/molxK	832.59	Joback Method
dvisc	0.0001222	Paxs	626.77	Joback Method

dvisc	0.0001577	Paxs	581.41	Joback Method
dvisc	0.0002123	Paxs	536.05	Joback Method
dvisc	0.0003021	Paxs	490.69	Joback Method
dvisc	0.0004619	Paxs	445.32	Joback Method
dvisc	0.0007775	Paxs	399.96	Joback Method
dvisc	0.0014954	Paxs	354.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R158091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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