

(3-Chloro-4-benzyloxy-phenyl)-propionic acid, methyl ester

Inchi:	InChI=1S/C17H17ClO3/c1-20-17(19)10-8-13-7-9-16(15(18)11-13)21-12-14-5-3-2-4-6-14
InchiKey:	QOSMQHRKFPWFKW-UHFFFAOYSA-N
Formula:	C17H17ClO3
SMILES:	COC(=O)CCc1ccc(OCc2ccccc2)c(Cl)c1
Mol. weight [g/mol]:	304.77

Physical Properties

Property code	Value	Unit	Source
gf	-53.03	kJ/mol	Joback Method
hf	-336.85	kJ/mol	Joback Method
hfus	35.26	kJ/mol	Joback Method
hvap	75.26	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.025		Crippen Method
mcvol	228.420	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	2332.30		NIST Webbook
rinpol	2332.30		NIST Webbook
tb	787.82	K	Joback Method
tc	1017.80	K	Joback Method
tf	483.54	K	Joback Method
vc	0.863	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.88	J/molxK	787.82	Joback Method
cpg	637.18	J/molxK	826.15	Joback Method
cpg	650.29	J/molxK	864.48	Joback Method
cpg	662.24	J/molxK	902.81	Joback Method
cpg	673.06	J/molxK	941.14	Joback Method
cpg	682.77	J/molxK	979.47	Joback Method
cpg	691.41	J/molxK	1017.80	Joback Method
dvisc	0.0005783	Paxs	483.54	Joback Method

dvisc	0.0003515	Paxs	534.25	Joback Method
dvisc	0.0002328	Paxs	584.97	Joback Method
dvisc	0.0001647	Paxs	635.68	Joback Method
dvisc	0.0001227	Paxs	686.39	Joback Method
dvisc	0.0000951	Paxs	737.11	Joback Method
dvisc	0.0000762	Paxs	787.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157954&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
hvap:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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