

(3-Chloro-4-cyclohexyloxy-phenyl)-acetic acid, methyl ester

Inchi:	InChI=1S/C15H19ClO3/c1-18-15(17)10-11-7-8-14(13(16)9-11)19-12-5-3-2-4-6-12/h7-9,1
InchiKey:	SLHLLQIFSNCBSX-UHFFFAOYSA-N
Formula:	C15H19ClO3
SMILES:	COC(=O)Cc1ccc(OC2CCCCC2)c(Cl)c1
Mol. weight [g/mol]:	282.76

Physical Properties

Property code	Value	Unit	Source
gf	-157.83	kJ/mol	Joback Method
hf	-477.78	kJ/mol	Joback Method
hfus	27.88	kJ/mol	Joback Method
hvap	68.96	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.767		Crippen Method
mcvol	213.140	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	2094.30		NIST Webbook
tb	734.93	K	Joback Method
tc	966.63	K	Joback Method
tf	441.96	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.47	J/molxK	734.93	Joback Method
cpg	612.81	J/molxK	773.55	Joback Method
cpg	628.80	J/molxK	812.16	Joback Method
cpg	643.47	J/molxK	850.78	Joback Method
cpg	656.83	J/molxK	889.39	Joback Method
cpg	668.89	J/molxK	928.01	Joback Method
cpg	679.66	J/molxK	966.63	Joback Method
dvisc	0.0009117	Paxs	441.96	Joback Method
dvisc	0.0005264	Paxs	490.79	Joback Method

dvisc	0.0003357	Paxs	539.62	Joback Method
dvisc	0.0002307	Paxs	588.45	Joback Method
dvisc	0.0001679	Paxs	637.27	Joback Method
dvisc	0.0001279	Paxs	686.10	Joback Method
dvisc	0.0001010	Paxs	734.93	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=R157994&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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