

3-Chlorobenzoic acid, cyclohexylmethyl ester

Inchi:	InChI=1S/C14H17ClO2/c15-13-8-4-7-12(9-13)14(16)17-10-11-5-2-1-3-6-11/h4,7-9,11H,1
InchiKey:	UEGFSNRJGAKXDY-UHFFFAOYSA-N
Formula:	C14H17ClO2
SMILES:	O=C(OCC1CCCCC1)c1cccc(Cl)c1
Mol. weight [g/mol]:	252.74

Physical Properties

Property code	Value	Unit	Source
gf	-51.62	kJ/mol	Joback Method
hf	-313.45	kJ/mol	Joback Method
hfus	24.49	kJ/mol	Joback Method
hvap	63.67	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.077		Crippen Method
mvol	193.180	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1959.00		NIST Webbook
rinpol	1959.00		NIST Webbook
tb	684.65	K	Joback Method
tc	923.52	K	Joback Method
tf	395.94	K	Joback Method
vc	0.718	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.71	J/mol×K	684.65	Joback Method
cpg	590.75	J/mol×K	883.71	Joback Method
cpg	578.12	J/mol×K	843.90	Joback Method
cpg	564.24	J/mol×K	804.09	Joback Method
cpg	549.08	J/mol×K	764.27	Joback Method
cpg	532.58	J/mol×K	724.46	Joback Method
cpg	602.18	J/mol×K	923.52	Joback Method
dvisc	0.0001479	Paxs	684.65	Joback Method

dvisc	0.0001901	Paxs	636.53	Joback Method
dvisc	0.0002546	Paxs	588.41	Joback Method
dvisc	0.0003592	Paxs	540.30	Joback Method
dvisc	0.0005422	Paxs	492.18	Joback Method
dvisc	0.0008946	Paxs	444.06	Joback Method
dvisc	0.0016673	Paxs	395.94	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=U357784&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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