

Octan-2-yl 3-chlorobenzoate

Inchi:	InChI=1S/C15H21ClO2/c1-3-4-5-6-8-12(2)18-15(17)13-9-7-10-14(16)11-13/h7,9-12H,3-6
InchiKey:	DRJCEVLJJXITPT-UHFFFAOYSA-N
Formula:	C15H21ClO2
SMILES:	CCCCCCC(C)OC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]:	268.78

Physical Properties

Property code	Value	Unit	Source
gf	-70.09	kJ/mol	Joback Method
hf	-393.69	kJ/mol	Joback Method
hfus	31.72	kJ/mol	Joback Method
hvap	65.08	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.856		Crippen Method
mcvol	218.130	ml/mol	McGowan Method
pc	1849.92	kPa	Joback Method
rinpol	1861.00		NIST Webbook
tb	687.54	K	Joback Method
tc	893.09	K	Joback Method
tf	384.83	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.17	J/molxK	687.54	Joback Method
cpg	592.04	J/molxK	721.80	Joback Method
cpg	606.95	J/molxK	756.06	Joback Method
cpg	620.94	J/molxK	790.31	Joback Method
cpg	634.03	J/molxK	824.57	Joback Method
cpg	646.24	J/molxK	858.83	Joback Method
cpg	657.61	J/molxK	893.09	Joback Method
dvisc	0.0015693	Paxs	384.83	Joback Method
dvisc	0.0007892	Paxs	435.28	Joback Method

dvisc	0.0004578	Paxs	485.73	Joback Method
dvisc	0.0002942	Paxs	536.18	Joback Method
dvisc	0.0002040	Paxs	586.64	Joback Method
dvisc	0.0001499	Paxs	637.09	Joback Method
dvisc	0.0001153	Paxs	687.54	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=U373684&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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