Decan-2-yl 3-chlorobenzoate

Inchi: InChI=1S/C17H25ClO2/c1-3-4-5-6-7-8-10-14(2)20-17(19)15-11-9-12-16(18)13-15/h9,11-
InchiKey: NNZBVJPJGGLPEB-UHFFFAOYSA-N
Formula: C17H25ClO2
SMILES: CCCCCCCCC(C)OC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 296.83

Physical Properties

Property code	Value	Unit	Source
gf	-53.25	kJ/mol	Joback Method
hf	-434.97	kJ/mol	Joback Method
hfus	36.90	kJ/mol	Joback Method
hvap	69.53	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.636		Crippen Method
mcvol	246.310	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	1968.00		NIST Webbook
tb	733.30	K	Joback Method
tc	934.38	K	Joback Method
tf	407.37	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.54	J/mol×K	733.30	Joback Method
cpg	702.08	J/mol×K	766.81	Joback Method
cpg	717.61	J/mol×K	800.33	Joback Method
cpg	732.18	J/mol×K	833.84	Joback Method
cpg	745.81	J/mol×K	867.35	Joback Method
cpg	758.53	J/mol×K	900.86	Joback Method
cpg	770.37	J/mol×K	934.38	Joback Method
dvisc	0.0013311	Pa×s	407.37	Joback Method
dvisc	0.0006521	Pa×s	461.69	Joback Method

dvisc	0.0003712	Pa×s	516.01	Joback Method
dvisc	0.0002353	Pa×s	570.34	Joback Method
dvisc	0.0001614	Pa×s	624.66	Joback Method
dvisc	0.0001176	Pa×s	678.98	Joback Method
dvisc	0.0000898	Pa×s	733.30	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=U373566&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