Decyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, decyl ester
Inchi: InChI=1S/C17H25ClO2/c1-2-3-4-5-6-7-8-9-13-20-17(19)15-11-10-12-16(18)14-15/h10-12
InchiKey: KJNHMQHNRBEWRN-UHFFFAOYSA-N
Formula: C17H25ClO2
SMILES: CCCCCCCCCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 296.83

Physical Properties

Property code	Value	Unit	Source
gf	-50.81	kJ/mol	Joback Method
hf	-429.69	kJ/mol	Joback Method
hfus	40.42	kJ/mol	Joback Method
hvap	69.92	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.638		Crippen Method
mcvol	246.310	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	2136.00		NIST Webbook
rinpol	2109.00		NIST Webbook
rinpol	2173.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2147.00		NIST Webbook
rinpol	2173.00		NIST Webbook
rinpol	2128.00		NIST Webbook
rinpol	2109.00		NIST Webbook
rinpol	2118.00		NIST Webbook
ripol	2669.00		NIST Webbook
ripol	2653.00		NIST Webbook
ripol	2689.00		NIST Webbook
ripol	2692.00		NIST Webbook
ripol	2658.00		NIST Webbook
ripol	2679.00		NIST Webbook
ripol	2653.00		NIST Webbook
tb	733.74	K	Joback Method
tc	931.90	K	Joback Method
tf	422.37	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.02	J/mol×K	733.74	Joback Method
cpg	701.30	J/mol×K	766.77	Joback Method
cpg	716.62	J/mol×K	799.79	Joback Method
cpg	731.01	J/mol×K	832.82	Joback Method
cpg	744.50	J/mol×K	865.85	Joback Method
cpg	757.11	J/mol×K	898.87	Joback Method
cpg	768.87	J/mol×K	931.90	Joback Method
dvisc	0.0011220	Pa×s	422.37	Joback Method
dvisc	0.0005974	Pa×s	474.26	Joback Method
dvisc	0.0003602	Pa×s	526.16	Joback Method
dvisc	0.0002378	Pa×s	578.06	Joback Method
dvisc	0.0001681	Pa×s	629.95	Joback Method
dvisc	0.0001253	Pa×s	681.85	Joback Method
dvisc	0.0000974	Pa×s	733.74	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=U373539&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume