Nonyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, nonyl ester
Inchi: InChI=1S/C16H23ClO2/c1-2-3-4-5-6-7-8-12-19-16(18)14-10-9-11-15(17)13-14/h9-11,13H
InchiKey: UKJRIERXEQWYQP-UHFFFAOYSA-N
Formula: C16H23ClO2
SMILES: CCCCCCCCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 282.81

Physical Properties

Property code	Value	Unit	Source
gf	-59.23	kJ/mol	Joback Method
hf	-409.05	kJ/mol	Joback Method
hfus	37.83	kJ/mol	Joback Method
hvap	67.69	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.247		Crippen Method
mcvol	232.220	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2019.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2021.00		NIST Webbook
rinpol	1971.00		NIST Webbook
rinpol	2033.00		NIST Webbook
ripol	2569.00		NIST Webbook
ripol	2553.00		NIST Webbook
ripol	2571.00		NIST Webbook
ripol	2549.00		NIST Webbook
ripol	2586.00		NIST Webbook
ripol	2590.00		NIST Webbook
tb	710.86	K	Joback Method
tc	910.76	K	Joback Method
tf	411.10	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.76	J/mol×K	710.86	Joback Method
cpg	645.71	J/mol×K	744.18	Joback Method
cpg	660.72	J/mol×K	777.49	Joback Method
cpg	674.83	J/mol×K	810.81	Joback Method
cpg	688.05	J/mol×K	844.12	Joback Method
cpg	700.42	J/mol×K	877.44	Joback Method
cpg	711.96	J/mol×K	910.76	Joback Method
dvisc	0.0012148	Pa×s	411.10	Joback Method
dvisc	0.0006558	Pa×s	461.06	Joback Method
dvisc	0.0003994	Pa×s	511.02	Joback Method
dvisc	0.0002657	Pa×s	560.98	Joback Method
dvisc	0.0001889	Pa×s	610.94	Joback Method
dvisc	0.0001415	Pa×s	660.90	Joback Method
dvisc	0.0001103	Pa×s	710.86	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373565&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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