Benzoic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C15H21ClO2/c16-12-8-3-1-2-4-9-13-18-15(17)14-10-6-5-7-11-14/h5-7,10-11H,
InchiKey: VRKHAMQZTBNMEV-UHFFFAOYSA-N
Formula: C15H21ClO2
SMILES: O=C(OCCCCCCCCCl)c1ccccc1
Mol. weight [g/mol]: 268.78

Physical Properties

Property code	Value	Unit	Source
gf	-58.02	kJ/mol	Joback Method
hf	-376.94	kJ/mol	Joback Method
hfus	35.63	kJ/mol	Joback Method
hvap	64.80	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.423		Crippen Method
mcvol	218.130	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2134.00		NIST Webbook
rinpol	2135.00		NIST Webbook
tb	683.00	K	Joback Method
tc	884.24	K	Joback Method
tf	387.31	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.27	J/mol×K	683.00	Joback Method
cpg	591.99	J/mol×K	716.54	Joback Method
cpg	606.78	J/mol×K	750.08	Joback Method
cpg	620.65	J/mol×K	783.62	Joback Method
cpg	633.65	J/mol×K	817.16	Joback Method
cpg	645.81	J/mol×K	850.70	Joback Method
cpg	657.15	J/mol×K	884.24	Joback Method

dvisc	0.0016280	Pa×s	387.31	Joback Method
dvisc	0.0008338	Pa×s	436.59	Joback Method
dvisc	0.0004891	Pa×s	485.87	Joback Method
dvisc	0.0003166	Pa×s	535.15	Joback Method
dvisc	0.0002205	Pa×s	584.44	Joback Method
dvisc	0.0001624	Pa×s	633.72	Joback Method
dvisc	0.0001251	Pa×s	683.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U367930&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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