3-Fluorobenzoic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C15H20ClFO2/c16-10-5-3-1-2-4-6-11-19-15(18)13-8-7-9-14(17)12-13/h7-9,12H
InchiKey: YZSYZDFQZYCLBT-UHFFFAOYSA-N
Formula: C15H20ClFO2
SMILES: O=C(OCCCCCCCCCCl)c1cccc(F)c1
Mol. weight [g/mol]: 286.77

Physical Properties

Property code	Value	Unit	Source
gf	-262.46	kJ/mol	Joback Method
hf	-584.52	kJ/mol	Joback Method
hfus	38.32	kJ/mol	Joback Method
hvap	64.65	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.562		Crippen Method
mcvol	219.900	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2122.00		NIST Webbook
rinpol	2122.00		NIST Webbook
tb	687.25	K	Joback Method
tc	881.81	K	Joback Method
tf	400.42	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.58	J/mol×K	687.25	Joback Method
cpg	598.51	J/mol×K	719.68	Joback Method
cpg	612.59	J/mol×K	752.10	Joback Method
cpg	625.83	J/mol×K	784.53	Joback Method
cpg	638.27	J/mol×K	816.96	Joback Method
cpg	649.93	J/mol×K	849.38	Joback Method
cpg	660.82	J/mol×K	881.81	Joback Method

Sources

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=U355666&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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