2,4-Difluorobenzoic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C15H19ClF2O2/c16-9-5-3-1-2-4-6-10-20-15(19)13-8-7-12(17)11-14(13)18/h7-8
InchiKey: FJUSSAQRWOUCMC-UHFFFAOYSA-N
Formula: C15H19ClF2O2
SMILES: O=C(OCCCCCCCCCl)c1ccc(F)cc1F
Mol. weight [g/mol]: 304.76

Physical Properties

Property code	Value	Unit	Source
gf	-466.90	kJ/mol	Joback Method
hf	-792.10	kJ/mol	Joback Method
hfus	41.01	kJ/mol	Joback Method
hvap	64.49	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.701		Crippen Method
mcvol	221.670	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpol	2068.00		NIST Webbook
rinpol	2068.00		NIST Webbook
tb	691.50	K	Joback Method
tc	880.08	K	Joback Method
tf	413.53	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.82	J/mol×K	691.50	Joback Method
cpg	605.04	J/mol×K	722.93	Joback Method
cpg	618.48	J/mol×K	754.36	Joback Method
cpg	631.14	J/mol×K	785.79	Joback Method
cpg	643.06	J/mol×K	817.22	Joback Method
cpg	654.26	J/mol×K	848.65	Joback Method
cpg	664.73	J/mol×K	880.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360562&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
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